Symmetry investigation of a generalised Lane-Emden equation of the second-kind

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Declaration

I declare that the contents of this thesis is original except where due references have been made. It has not been submitted before for any degree to any other institution.

C. Harley

Dedication

I dedicate this thesis to my mother and father.

Acknowledgements

I would like to thank my supervisor, Prof. E. Momoniat, for all his guidance and support. I would also like to offer my gratitude to the members of the School of Computational and Applied Mathematics, especially Prof. F.M. Mahomed and Prof. D.P. Mason, for all their help and advice. I also sincerely appreciate all the useful discussions with Prof. A. Qadir.

Abstract

In this thesis a Lane-Emden equation of the second-kind is investigated. The equation is considered with arbitrary parameters with the intention of obtaining a solution without referring to specific cases. The shape factor is a parameter indicating the type of vessel relevant to the physical problem considered. There are various forms of the equation. We will consider two such forms, where the shape factor is specified to be one and two, which are of some physical significance. One of these equations is derived from the steady state heat balance equation, and in so doing models a thermal explosion. The other equation that is of importance is derived from equations of mass conservation and dynamic equilibrium. This gives a model describing the dimensionless density distribution in an isothermal gas sphere. This equation when transformed appropriately may also be used to model Bonnor-Ebert gas spheres or Richardson's theory of thermionic currents which is related to the emission of electricity from hot bodies. Lie's theory of extended groups is used in order to obtain infinitesimal generators and in association with Noether's theorem may be used to find appropriate first integrals of the equation. Non-local symmetries are used in conjunction with local symmetries in order to verify already obtained solutions and to obtain new solutions. For specified values of the shape factor solutions were obtained in this way within an infinite slab, infinite circular cylinder and sphere. Computational methods, such as finite differences, are used to obtain new numerical solutions which are useful indicators for the exactness of the solutions obtained via other means. We were unable to obtain solutions to certain specific cases because of the nature of the equation in question. New physical and mathematical insights are revealed through the solutions found and the comparisons made between them and other already existing solutions.

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Chapter 1

Introduction

The main purpose of this thesis is to contribute to the known solutions of the Lane-Emden equation of the second-kind. This is done mainly through the use of Lie's theory of extended groups, [55, 13, 43, 44], Noether symmetries [53] and Non-local symmetries, [2, 3]. We consider a Lane-Emden equation of the second-kind, with parameters δ and k. The critical exponent, δ, is also known as the Frank-Kamenetskii [29] parameter. The value of k determines the shape of the vessel within which the process modelled by the equation occurs and hence is referred to as the shape factor. For well defined geometries $k = 0$ represents an infinite slab, $k = 1$ an infinite circular cylinder and $k = 2$ a sphere. Balakrishnan et al. [9] shows that there are shapes that do not have integer values for k. In this thesis we will be considering the well-defined geometries referred to above, and also aim to obtain appropriate solutions for all values of k.

Processes which pertain to astronomy and chemistry can be modelled by the second-order ordinary differential equation considered in this thesis. One of the two physical systems that we will investigate is derived via the equations for mass conservation and dynamic equilibrium. In the study of stellar structures one considers the star as a gaseous sphere in thermodynamic and hydrostatic equilibrium with a certain equation of state. The gravitational equilibrium of a gaseous configuration in which the pressure and density accelerated was first considered by Lane [48], and then independently considered by Ritter [59] and Kelvin [64]. In particular, the equation of state for polytropic gas spheres was proposed by Lane and then studied in detail by Emden [27], on whose work the derivation of the equation we consider in this thesis is based. The interested reader is also referred to the books by [12] and [47].

The work referred to in the above paragraph lead to the development of a Lane-Emden equation of the second-kind capable of modelling the dimensionless density distribution of isothermal gas spheres, and with the appropriate transformations Bonnor-Ebert gas spheres [15] and Richardson's theory of thermionic currents [58] which is related to the emission of electricity from hot bodies. Since the geometry relevant to this physical system is that of a sphere the shape factor k is defined as two. The initial conditions reflect the symmetry of the density distribution at the central axis $x = 0$ and maintain an initial density of zero.

Chandrasekhar [22] considered the mathematical problem of determining the structure of an equilibrium configuration in which the pressure and density of a polytropic sphere are related. Chandrasekhar [22] determined a power series solution admitted by the Lane-Emden equation when it models the dimensionless density distribution in a sphere, solved subject to the initial conditions mentioned above. Wazwaz [67] has used the Adomian decomposition method to determine a power series solution for the same equation. Relevant transformations can be made to this solution to obtain solutions that can be applied to Bonnor-Ebert gas spheres and Richardson's theory of thermionic currents [58]. Nouh [54] accelerated the convergence of the power series solution by using an Euler-Abel transformation and a Padè approximation. Liu [49] obtained a different power series solution for the same system. Ramos [57] proved that the convergence of the standard power series solution of the Lane-Emden equation is valid for $|x^2| < 1$. A physical interpretation for this radius of convergence has been given by Hunter [41], who in fact has also shown how the radius of convergence can be increased by means of an Euler transformation of the Lane-Emden equation.

The second physical system which we focus our attention on is one which considers the temperature distribution in different geometries. In this system the constant δ is an eigenvalue representing the critical temperature for a thermal explosion. We consider in particular the phenomena of combustion occurring within an infinite rectangular slab and an infinite circular cylinder. The relevant form of the Lane-Emden equation of the second-kind is derived from the heat balance equation. Frank-Kamenetskii [29] is mainly responsible for a steady state formulation of this system. We consider a thermal explosion due to a chemical reaction in a cylindrical vessel with boundary conditions that ensure continuity at the centre of the vessel and fixes the non-dimensional temperature at the wall. For the infinite slab the temperature is fixed at the boundaries.

Steady state solutions for a thermal explosion in a cylindrical vessel have been obtained by Frank-Kamenetskii [29] who transformed the Lane-Emden equation describing this physical process into a second-order autonomous ordinary differential equation. The resulting second-order ordinary differential equation is solved and an analytical solution is obtained. Frank-Kamenetskii [29] analytically determines the critical value of δ for $k = 0$ and $k = 1$. Chambré [21] uses a differential invariant to reduce the equation to a first-order ordinary differential equation. The resulting first-order ordinary differential equation is solved and a solution satisfying the boundary conditions, mentioned in the above paragraph, is obtained for $k = 0$ and $k = 1$. Barrenblatt [10] numerically obtains the temperature distribution in a cylindrical vessel in which the vessel walls are periodically thermally conducting. The self-ignition of a chemically active mixture of gasses in a plane, cylinder and spherical vessel is considered by Gelfand [32]. Balakrishnan et al. [9] shows that there are shapes that do not have integer values for k and has solved the associated Lane-Emden equation numerically for these non integer values of k. In his work the value of k is dependent on other variables such as the volume of the body and the surface area. He considered in particular the infinite square rod and cube.

A lot more work has been done on thermal explosions in a square vessel, [29, 63, 26], due to the ease with which analytical solutions can be obtained and analyzed. Dumont et al. [26] include the effects of convection on a thermal explosion in a two dimensional square vessel. Combustion occurring from a single point has been well studied from a partial differential equation perspective, [20, 30, 40, 51, 65, 66, 31].

The existence and uniqueness of solutions of the Lane-Emden equation with parameters δ and k subject to the boundary conditions required for the thermal explosion in a vessel has been proved by Russell and Shampine [60]. They develop three numerical approaches to solving singular boundary value problems of this form. The interested reader is referred to Shampine et al. [61] for more information on using the MATLAB program `bvp4c` to solve boundary value problems.

An outline of this thesis is as follows. A brief overview is given in Chapter 2 on the theory of Lie group analysis, [55, 13, 43]. The uses of local and non-local Lie group analysis, [2, 3], are explained in reference to our work and we also discuss the import of using Noether symmetries, [53]. The numerical techniques that are used are not discussed here but referred to in the appropriate Chapters.

In Chapter 3 we use the Lie group method, [13, 44], to reduce the Lane-Emden equation which models the dimensionless density distribution to a first-order ordinary differential equation. We are unable to determine an analytical solution admitted by the reduced equation. Instead, we obtain a power series solution admitted by the reduced equation which transforms into an approximate implicit solution of the equation considered. In this manner we have improved on the accuracy of the power series obtained by Chandrasekhar [22] by considering a power series solution of a first-order reduction of the Lane-Emden equation of the second-kind. The resulting power series solution has a larger radius of convergence than the power series solution of Chandrasekhar [22].

We use the theory of Lie, [55, 13, 43], in Chapter 4 to determine differential invariants that reduce the Lane-Emden equation with shape factor one to first-order. A new parametric solution admitted by the reduced first-order equation is obtained. Using the direct method of Adam and Mahomed [2, 3] we determine a non-local symmetry admitted by the reduced equation producing a solution that describes the ignition occurring within the vessel. Relationships between the parameter δ and the boundary conditions for the thermal explosion problem are obtained. This is done via Noether's theorem which is used to determine first integrals admitted the by equation for critical exponents zero and one. In this way the well known critical value for the Frank-Kamenetskii [29] parameter, $\delta = 2$, is obtained without first needing to solve the ordinary differential equation .

In Chapter 5 we investigate the invariant boundary conditions of the Lane-Emden equation of the second-kind. We use the Lie point symmetry group generators admitted by the equation to obtain these invariant boundary conditions as discussed in Bluman and Kumei [13]. The stability of the boundary condition $y' = 0$ on the line $x = 0$ is analysed by investigating phase diagrams of a reduced equation. We demonstrate the instability of the boundary condition $y' = 0$ on the line $x = 0$ by considering a numerical solution using `bvp4c` in MATLAB and propose how this instability can be overcome.

In Chapter 6 a perturbation is introduced into the Lane-Emden equation. By imposing the boundary conditions for the thermal explosion problem on the first integrals, obtained through the use of Noether's theorem, admitted by the perturbed equation we obtain a nonlinear relationship between the temperature at the center of the vessel and the temperature gradient at the wall of the vessel. For a rectangular slab the presence of a bifurcation indicates multivalued solutions for the temperature at the center of the vessel when the temperature gradient at the wall is fixed. For a cylindrical vessel we find a bifurcation indicating multivalued solutions for the temperature gradient at the walls of the vessel when the temperature at the center of the vessel is fixed.

In Chapter 7 we determine a power series solution of a reduced first-order Abel equation equation found by using a coordinate transformation introduced by Chandrasekhar [22] to reduce the Lane-Emden equation of the second-kind to autonomous form. When converting back to the original variables the power series solution transforms into an implicit series solution of the equation. The boundary conditions are easily imposed on this implicit series solution. Numerical comparisons are made between the newly obtained implicit series solution and solutions obtained in previous

Chapters.

In the final Chapter the conclusions drawn from the work done in this thesis are summarised.

Chapter 2

Physical derivation, Lie Group Method, Noether's theorem and Non-local symmetries

In this Chapter we describe two derivations of the Lane-Emden equation of the second-kind pertaining to two physical systems. We also review the general theory related to local and non-local one-parameter group transformations. A brief discussion of Noether's theorem is included. Work done by Clèment et al. [24] on a quasilinear differential equation and the Lie point symmetry group generator thereof is briefly noted in the last Section.

2.1 Physical derivation of the equations

The equation we consider in this thesis has two important ways in which it may be derived. We consider these methods since our research stems from the investigation of these physical systems. One model is derived through the investigation of the equations of mass conservation and dynamic equilibrium. It describes the density distribution of isothermal gas spheres, Bonnor-Ebert gas spheres [15] and Richardson's theory of thermionic currents [58] by specifying the geometry of the vessel in an appropriate fashion. The second model is derived from the heat balance equation and describes the temperature distribution in different geometries. The blow-up that takes place in these geometries has various interesting properties reflected by solutions found.

2.1.1 The density distribution in a sphere

The model we consider here originates from work done in particular by Chandrasekhar [22]. In his investigations he considered stars which are in equilibrium and which are in a steady state. Chandrasekhar [22] maintains that the equilibrium configuration of these stars can be characterized by three parameters: its the mass, M; its radius, r; and its luminosity, L. The luminosity is defined as being the amount of radiant energy radiated by the star per second to the space outside. It specifies the net flux of energy given by $L/4\pi R^2$ at the boundary of the star. Another assumption made concerning the density distribution of a star is that the distribution is such that the mean density $\bar{\rho}(r)$, interior to the given point r inside the star, does not increase outward from the center.

We will be considering an isothermal gas sphere, where we find that the pressure, P and the spatial density, ρ are related as follows,

$$P = K\rho + D \tag{2.1}$$

where K and D are constants, dependent on the thermodynamic properties of the isothermal gas sphere. For example in Chavanis [23] the constants K and D are related to physical properties of finite isothermal spheres.

This relationship stems from equations of gravitational equilibrium which we consider in order to attain a Lane-Emden equation of the second-kind able to describe the dimensionless density distribution in an isothermal gas sphere. We let r denote the radius measured from the center of the configuration. Since we consider in particular isothermal gas spheres we are concerned with spherical symmetrical distributions of matter. This leads to the conclusion that the total pressure, P, the spatial density, ρ, and other physical variables will be functions of r only, [22]. We consider the equation of mass conservation

$$\frac{dM}{dr} = 4\pi r^2 \rho(r) \tag{2.2}$$

with $M(r)$ the mass of the star at a distance r from the center of the star. As defined above $\bar{\rho}(r)$ denotes the mean density inside r, whereas $\bar{\rho}$ describes the mean density for the whole configuration as follows [22]

$$\bar{\rho}(r) = \frac{M(r)}{\frac{4}{3}\pi r^3}, \qquad \bar{\rho} = \frac{M}{\frac{4}{3}\pi R^3} \tag{2.3}$$

where M is the mass of the configuration and R defines the radius thereof at which ρ and P vanish. The equation governing the dynamic equilibrium of the configuration is given by

$$\frac{dP}{dr} = -\frac{M(r)\rho(r)G}{r^2} \tag{2.4}$$

where P denotes the total pressure at radius r, G is the constant of gravitation and $\rho(r)$ the spatial density at a distance r from the centre of the star. When combining equations (2.2) and (2.4) we obtain Poisson's equation

$$\frac{1}{r^2}\frac{d}{dr}\left(\frac{r^2}{\rho(r)}\frac{dP}{dr}\right) = -4\pi G\rho. \tag{2.5}$$

To produce a Lane-Emden equation of the second-kind we consider the substitutions

$$\rho = \rho_c e^{-y}, \qquad r = \left[\frac{K}{4\pi G\rho_c}\right]^{1/2} x \tag{2.6}$$

where ρ_c is defined to be the central density. It is noted that the central density is also the maximum density at $r = 0$ since the density decays from the center of the star in an outwardly direction as indicated by the substitution $\rho = \rho_c e^{-y}$. Substituting (2.1) into (2.2) and (2.4) and using the transformations mentioned above (2.6) reduces the second-order ordinary differential equation (2.5) to the Lane-Emden equation of the second-kind,

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{dy}{dx}\right) = e^{-y} \tag{2.7}$$

which describes the dimensionless density distribution in an isothermal gas sphere. Equation (2.7) is a more compact version of equation (2.28), derived in the next Section, with $k = 2$. A lower bound on the ratio $\rho/\rho_c > 1/32.1$ from (2.6) is obtained by Chavanis [23] for the stability of finite isothermal spheres.

2.1.2 A thermal explosion within a vessel

The mathematical theory of combustion according to Frank-Kamenetskii [29] deals with the combined systems of equations of chemical kinetics and of heat transfer and diffusion. The reaction rate depends on the temperature in a nonlinear fashion, generally given by Arrhenius' law. This nonlinearity is an important characteristic of the combustion phenomena since without it the critical condition for inflammation would disappear causing the idea of combustion to lose its meaning [29]. From these premises the equation of combustion theory, neglecting the dependence of the thermal conductivity on the temperature, is given by [29]

$$\frac{\partial T}{\partial t} = a\nabla^2 T + \frac{Q}{c_p \rho} W(T) \tag{2.8}$$

which takes account of a continuous distribution of heat sources of density QW, where Q is the heat of the reaction and W is the reaction rate or velocity. We have defined a to be the thermal diffusivity of the mixture of gasses, T the gas temperature, c_p the mean mass heat capacity of the mixture at constant pressure and ρ the density with ∇^2 the Laplacian operator. The heat capacity c_p is a measure of the heat energy required to increase the temperature of a unit quantity of the gas by a certain temperature interval. More heat energy is required to increase the temperature of the gas with high specific heat capacity than one with low specific heat capacity. The reaction rate W is defined according to Arrhenius' law so that

$$W = \kappa\alpha e^{-(E/RT)} \tag{2.9}$$

where κ is the concentration of the reactant, α the frequency factor and E the energy of activation of the reaction. If we write $\lambda = c_p \rho a$, defined as the thermal conductivity of the mixture, then equation (2.8) can be rewritten in the form

$$\frac{1}{a}\frac{\partial T}{\partial t} = \nabla^2 T + \frac{Q}{\lambda}\kappa\alpha e^{-(E/RT)}. \tag{2.10}$$

This equation is subject to certain boundary conditions given at the walls of the vessel. The constant temperature T_0 is used at the internal surface of the walls.

At some particular value of the temperature the stationary distribution becomes impossible. This temperature is assumed to be the inflammation temperature and referred to as the critical condition. Since the stationary distribution in the reacting system becomes impossible at some critical condition it is important to transform the equation into a dimensionless state. To obtain dimensionless variables appropriate as transformations for equation (2.10) we consider the combustion phenomena quantitatively. We expand the exponential term of the Arrhenius expression as follows [29]

$$\frac{E}{RT} = \frac{E}{R(T_0 + \Delta T)} = \frac{E}{RT_0}\left[\frac{1}{1+\frac{\Delta T_0}{T_0}}\right] = \frac{E}{RT_0}\left[1 - \frac{\frac{\Delta T}{T_0}}{1+\frac{\Delta T}{T_0}}\right] \tag{2.11}$$

where $\Delta T = T - T_0$. From here we may write that

$$-\frac{E}{RT} = -\frac{E}{RT_0} - \frac{\theta}{1+\epsilon\theta} \tag{2.12}$$

where θ is defined as the dimensionless temperature difference

$$\theta = \frac{E}{R{T_0}^2}(T - T_0). \tag{2.13}$$

Hence the exponential term for the reaction rate W can be given exactly as

$$e^{-\frac{E}{RT}} = e^{-\frac{E}{RT_0}} e^{\frac{\theta}{1+\epsilon\theta}} \tag{2.14}$$

where $\epsilon = \frac{RT_0}{E}$ is introduced as a dimensionless parameter. To be able to speak of combustion the condition $\epsilon \ll 1$ must be satisfied, [29]. This is due to the fact that T_0 can normally be seen as much smaller in magnitude than the ignition temperature.

By substituting into equation (2.10) the expression given by (2.14) and using the dimensionless temperature difference θ defined by (2.13) the following equation is obtained [29, 21]

$$\frac{1}{a}\frac{\partial\theta}{\partial t} = \nabla^2\theta + \left[\frac{Q}{\lambda}\frac{E}{R{T_0}^2}\kappa\alpha e^{-(E/RT_0)}\right] e^{\theta/(1+\epsilon\theta)}. \tag{2.15}$$

Since the theory applied here is for geometries where the conduction process depends on only one space coordinate, say x, the Laplacian operator is made dimensionless by replacing the space coordinate x by $z = x/r$. By rescaling time t we obtain the following equation where the Laplacian operator is non-dimensional

$$\frac{\partial \theta}{\partial t} = \nabla^2 \theta + \delta e^{\theta/(1+\epsilon\theta)} \tag{2.16}$$

and the Frank-Kamenetskii parameter δ is given by

$$\delta = \frac{Q}{\lambda} \frac{E}{R{T_0}^2} r^2 \kappa \alpha e^{\left(-\frac{E}{RT_0}\right)}. \tag{2.17}$$

The Laplacian operator has now taken the form

$$\nabla^2 = \frac{d^2}{dz^2} + \left(\frac{N-1}{z}\right)\frac{d}{dz}, \qquad 0 < z < 1 \tag{2.18}$$

where N indicates the shape of the vessel within which the chemical reaction takes place. $N = 1, 2$ and 3 represents an infinite slab, infinite circular cylinder and sphere, respectively. In Figure 2.1 the geometries of $N = 1$ and $N = 2$ are shown.

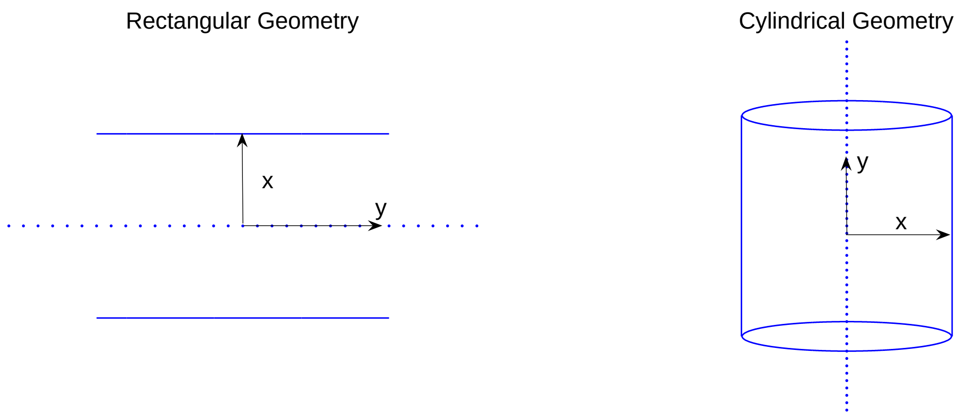

Figure 2.1: *Figure showing rectangular and cylindrical geometry.*

The explicit dependence of the model equation (2.16) on the Frank-Kamenetskii parameter δ can be removed by making a further change of variables

$$u = \theta - \theta_0, \qquad x = z\left[\delta e^{\theta_0}\right]^{1/2} \tag{2.19}$$

where θ_0 is the dimensionless temperature at the vessel walls. Through these transformations (2.19) the explicit dependence of the steady state model equation (2.16) on the Frank-Kamenetskii parameter δ is removed. Then by rescaling time t, ignoring coefficients $O(\epsilon)$, thus applying the Frank-Kamenetskii approximation $\epsilon \ll 1$, (2.16) is written as

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{k}{x}\frac{\partial u}{\partial x} + e^u \tag{2.20}$$

where $k = N - 1$ is a constant known as the shape factor. The model equation (2.16) is solved subject to

$$u(x,0) = \text{constant} = \theta_0, \tag{2.21}$$

$$\frac{\partial u}{\partial x}(0,t) = 0, \qquad u(R,t) = -\theta_0 \tag{2.22}$$

where

$$R = \left[\delta e^{\theta_0}\right]^{1/2}. \tag{2.23}$$

We note here that the dependence on δ is now in the boundary condition. The equation (2.20) describes a thermal explosion in a cylindrical vessel and the boundary conditions (2.21) and (2.22) imply that the temperature at the vessel walls are kept fixed and the solution is symmetric about the origin. The value of the Frank-Kamanetskii parameter [29] δ is related to the critical temperature at which ignition in a thermal explosion takes place and is this also referred to as the critical value.

The steady state formulation of the problem (2.8) is due essentially to Frank-Kamenetskii [29]. It has been postulated in the theory of thermal explosions that the critical condition for inflammability is reached when the amount of heat that has accumulated due to the chemical reaction is equal to the amount lost to the surroundings [21]. Frank-Kamenetskii [29] proposed a model where the loss of heat to the vessel walls, which must be in balance with the chemical heat being released, takes place entirely by conduction inside the gas volume. If this is the case then a certain temperature distribution in the mixture of gasses within the vessel will be obtained. The highest temperature will be at the center of the vessel where inflammation should theoretically start [29]. Since the theory of ignition states that an exothermic reaction which loses heat to the surroundings can achieve steady state only under certain conditions, there is a critical value above which no steady state is possible and explosion or ignition must occur, [9]. Hence after inflammation a stationary temperature distribution becomes impossible. One of the models Frank-Kamenetskii [29] proposed assumes that there is no convection and is considered with conduction only, [29].

A steady state formulation of the problem described by (2.16) can be given by the Poisson-Boltzmann equation [21]

$$\frac{d^2\theta}{dz^2} + \frac{k}{z}\frac{d\theta}{dz} = -\delta e^{\theta} \tag{2.24}$$

where the boundary condition at the center of the vessel

$$z = 0, \qquad \frac{d\theta}{dz} = 0 \tag{2.25}$$

is due to symmetry. At the wall of the vessel the boundary condition

$$z = 1, \qquad \theta = 0 \tag{2.26}$$

is required to fix the temperature.

To gain such steady state solutions admitted by (2.20) we assume the following form for the solution

$$u(x,t) = y(x). \tag{2.27}$$

The model equation (2.20) then reduces to the second-order ordinary differential equation

$$y'' + \frac{k}{x}y' + e^{y} = 0 \tag{2.28}$$

where $' = d/dx$. Equation (2.28) is a Lane-Emden equation of the second-kind. The boundary conditions (2.22) reduce to

$$y'(0) = 0, \qquad y\,(R) = -\theta_0. \tag{2.29}$$

For later analysis we retain the parameters ϵ and δ in our model for steady state solutions by letting $\theta = y$ and $N = k+1$ so that equation (2.16) reduces to (2.30).

$$y'' + \frac{k}{x}y' + \delta \exp\left(\frac{y}{1+\epsilon y}\right) = 0, \qquad \epsilon \ll 1. \tag{2.30}$$

This equation gives the opportunity to study the steady state heat balance equation where the parameter ϵ acts as a perturbation parameter.

2.2 Lie group method

There has been an explosion of advances in symmetry methods (group analysis) of differential equations, since the investigations done by Sophus Lie [43]. This is probably due to the applicable nature of the methods to nonlinear differential equations. Lie [13] developed highly algorithmic symmetry methods in order to unify and extend various specialized solution methods for ordinary differential equations. If an ordinary differential equation is invariant under a one-parameter Lie group of point transformations then the order of the ordinary differential equation can be reduced constructively. Elementary examples of Lie groups [13] include translations, rotations and scalings. The following theory is contained in the works by Bluman and Kumei [13] and Ibragimov [43].

In order to illustrate the power of the Lie group method we will look at a second-order ordinary differential equation

$$F(x, y, y', y'') = 0. \tag{2.31}$$

The Lie group approach considers a local transformation of the dependent and independent variables of the differential equation under consideration. We consider invertible transformations of the (x, y) plane

$$\overline{x} = \varphi(x, y, a), \qquad \overline{y} = \psi(x, y, a) \tag{2.32}$$

which depend upon a real parameter a, where we impose the conditions

$$\varphi|_{a=0} = x, \qquad \psi|_{a=0} = y. \tag{2.33}$$

These transformations are said to form a one-parameter group G if the successive action of two transformations is equivalent to the action of another transformation of the form given by (2.32). It can happen that this property is only valid locally and in this case G is referred to as a local one-parameter transformation group. The transformations given by (2.32) are called point transformations. When the transformed values also depend on the derivative y' then they are referred to as contact transformations.

The Taylor series expansions of the local transformations represented by the functions φ and ψ with respect to the parameter a in the neighbourhood of $a = 0$ provides us with the infinitesimal transformations

$$\overline{x} \approx x + a\xi(x, y), \qquad \overline{y} \approx y + a\eta(x, y). \tag{2.34}$$

The infinitesimal operator of the one-parameter Lie group of transformations (2.34) is the first-order differential operator

$$X = \xi(x, y)\frac{\partial}{\partial x} + \eta(x, y)\frac{\partial}{\partial y} \tag{2.35}$$

where

$$\xi(x, y) = \frac{\partial \varphi(x, y, a)}{\partial a}|_{a=0}, \qquad \eta(x, y) = \frac{\partial \psi(x, y, a)}{\partial a}|_{a=0}. \tag{2.36}$$

We are considering an equation (2.31) which is second-order, i.e. it is a function of the variables y' and y'' as well as x and y, thus the infinitesimal generator (2.35) must be prolonged (extended) to account for the additional variables y' and y''. A second-order prolongation (extension) of (2.35) is given by

$$X^{[2]} = X + \zeta^{(1)}\frac{\partial}{\partial y'} + \zeta^{(2)}\frac{\partial}{\partial y''} \tag{2.37}$$

where

$$\zeta^{(1)} = \eta_x + (\eta_y - \xi_x)y' - \xi_y y'^2, \tag{2.38}$$

$$\zeta^{(2)} = \eta_{xx} + (2\eta_{xy} - \xi_{xx})y' + (\eta_{yy} - 2\xi_{xy})y'^2 - \xi_{yy}y'^3 + (\eta_y - 2\xi_x)y'' - 3\xi_y y'y'' \tag{2.39}$$

where subscripts denote differentiation, [13].

From Bluman and Kumei [13] a function $F(x)$ which is infinitely differentiable is an invariant function of the Lie group of transformations (2.32) if an only if for any group transformation (2.32)

$$F(\overline{x}, \overline{y}) = F(x, y). \tag{2.40}$$

In turn the function $F(x)$ is an invariant of the group G with the symbol X (2.35) if and only if is satisfies the partial differential equation

$$XF \equiv \xi(x, y)\frac{\partial F}{\partial x} + \eta(x, y)\frac{\partial F}{\partial y}. \tag{2.41}$$

If an ordinary differential equation admits the group G then the frame of the equation is invariant [43] as discussed in the above paragraph. However if the ordinary differential equation in question (2.31) is a second-order ordinary differential equation then the equation will admit a group G if its frame is invariant under the second prolongation. As a consequence if the transformations (2.34) leave the equation under consideration form invariant, we can write (2.31) as

$$F\left(\overline{x}, \overline{y}, \frac{d\overline{y}}{d\overline{x}}, \frac{d^2\overline{y}}{d\overline{x}^2}\right) = 0. \tag{2.42}$$

Using the second prolongation of the infinitesimal generator (2.35) given by (2.37) the partial differential equation (2.41) can be satisfied for this equation.

The coefficients ξ and η of the infinitesimal generator (2.35) are determined by solving the determining equation

$$X^{[2]}F(x, y, y', y'')\big|_{y''=G(x,y,y')} = 0. \tag{2.43}$$

Expanding (2.43) we get

$$\xi F_x + \eta F_y + \zeta^{(1)} F_{y'} + \zeta^{(2)} F_{y''}\big|_{y''=G(x,y,y')} = 0. \tag{2.44}$$

The terms $\zeta^{(1)}$ and $\zeta^{(2)}$ from (2.38) and (2.39) are substituted into (2.44). Since ξ and η are functions of x and y only, the resulting equation can be separated by coefficients of powers of y' to obtain an over-determined linear system of equations for ξ and η. The resulting system of equations is then solved to give ξ and η as functions of x and y which we then use to obtain the infinitesimal generator (2.35) admitted by (2.31).

A group invariant solution $y = \Phi(x)$ admitted by (2.31) corresponding to the infinitesimal generator (2.35) is calculated by solving the first-order ordinary differential equation obtained from [44],

$$X\left(y - \Phi(x)\right)\big|_{y=\Phi(x)} = 0. \tag{2.45}$$

This will reduce the order of equation (2.31) producing a first-order ordinary differential equation. Bluman and Kumei [13] discuss different ways of determining the invariant solution.

Lie point symmetries admitted by differential equations are easily calculated by using computer algebra packages like MathLie [11] or Lie [39, 62]. The interested reader is referred to Bluman and Kumei [13] and Ibragimov [44] for more information on the application of Lie group analysis to differential equations.

2.3 Noether symmetries

The concept of a conservation law has historically been very prevalent in physics. This is motivated by the conservation of such quantities as energy, linear and angular momentum, etc. for equations that arise in classical particle mechanics [43]. It has been known for a long time that the conservation laws of classical mechanics are connected with symmetry properties of the physical system. However Noether (1918) [53] was the first to combine methods from variational calculus with Lie group theory and to formulate a general approach for constructing conservation laws for Euler-Lagrange equations when their symmetries are known. Thus she showed that it is more fruitful if one considers transformations which leave the action integral $J(u) = \int_\Omega L dx$ with L as the Lagrangian of the equation invariant [13]. This connection between invariances and conservation laws is now formalised by what is known as Noether's theorem. Thus a relationship between symmetries and Lagrangians admitted by an equation has been developed which enables us to understand and generate the first integrals of the equation.

Noether's theorem [53] states that if we can find an operator X given by

$$X = \xi \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y} \tag{2.46}$$

where

$$X(L) + L D_x \xi = D_x B \tag{2.47}$$

where D_x is the operator of total differentiation given by

$$D_x = \frac{\partial}{\partial x} + y' \frac{\partial}{\partial y} + y'' \frac{\partial}{\partial y'} + \cdots \tag{2.48}$$

and L is a solution of the Euler-Lagrange equation

$$\frac{d}{dx}\frac{\partial L}{\partial y'} - \frac{\partial L}{\partial y}\bigg|_{(2.46)} = 0 \tag{2.49}$$

with B as a gauge term then

$$I = L\xi + (\eta - \xi y')\,\frac{\partial L}{\partial y'} - B \tag{2.50}$$

is a first integral of the equation under consideration. The operator X is then known as a Noether or variational symmetry of the Lagrangian.

As shown above ordinary differential equations such as equation (2.31) can also be written in reduced form through conservation laws. This *conserved quantity* (2.50) of the Euler-Lagrangian equation satisfies the following properties

$$D_x I = 0, \qquad X^{[2]} I = 0. \tag{2.51}$$

Thus we can determine a solution to equation (2.31) by solving

$$I = c \tag{2.52}$$

where c is a constant.

Bluman [14] and Anco and Bluman [5, 6, 7] introduced the Direct Construction Method to determine conservations laws or first integrals of systems of equations that do not possess a Lagrangian formulation. Kara and Mahomed [46] have investigated the relationship between symmetries and conservation laws. They have determined a formula from which symmetries of conservation laws can be constructed without recourse to a Lagrangian. Feroze and Kara [28] developed the notion of an approximate Lagrangian and an approximation to Noether's theorem to obtain approximate first integrals.

2.4 Non-local symmetries

Noether's theorem and the Lie group-theoretic approach used to solve scalar first-order ordinary differential equations are well known. However, often finding these symmetries can be a problem due to the difficulty in solving the determining equations. This possible complexity has caused non-local symmetries to receive the attentions of many and consequently they have been investigated for quite some time now [4].

Consider a second-order ordinary differential equation which admits an algebra L_2 of generators of point symmetries in a suitable basis $\{X_1, X_2\}$ such that $[X_1, X_2] = kX_1$, for $k \neq 0$ constant. If the reduction of this equation is via a symmetry which does not span an ideal of the algebra L_2, viz. X_2 then X_1 is lost as a point symmetry of the reduced first-order equation. It becomes a *non-local symmetry* [2, 3]. Adam and Mahomed [2, 3] have developed a method of canonical variables by means of which an exponential non-local symmetry of the reduced first-order equation is mapped to a canonical exponential non-local symmetry thereby simplifying the transformed equation to an integrable form. In this way they, [2, 3], have developed a direct method for determining non-local symmetries admitted by a second-order ordinary differential equation from its symmetry reduction. This method can basically be summarised into a four-step algorithm:

Step one: We convert the first-order ordinary differential equation to be solved

$$H(u, v) = \frac{dv}{du} \tag{2.53}$$

into a second-order ordinary differential equation

$$F(x, y, y') = y'' \tag{2.54}$$

by means of the invariants

$$u = u(x, y), \qquad v = v(x, y, y') \tag{2.55}$$

of a point symmetry X_1 of (2.54).

Step two: Another point symmetry X_2 of (2.54) is found such that $\{X_1, X_2\}$ spans a two-dimensional Lie algebra.

Step three: If necessary introduce a basis so that $[X_1, X_2] = X_2$.

Step four: X_2 then becomes an exponential non-local symmetry in terms of (u, v)

$$\tilde{X}_2 = exp\left(\int N(u, v)du\right)\left(\xi(u)\frac{\partial}{\partial_u} + \eta(u, v)\frac{\partial}{\partial_v}\right). \tag{2.56}$$

Now find a transformation $(u, v) \mapsto (U, V)$ that reduces (2.53) to an integrable form. There are two possibilities.

(i) If $X_1 \neq \rho(x, y)X_2$ for any function ρ, then

$$U = a(u), \qquad V = a(u) - \frac{a'(u)}{\alpha} \tag{2.57}$$

where $\alpha = N + \frac{a''}{a'} + \frac{\xi_u}{\xi}$ and $a(u)$ is a solution of

$$a\xi\alpha^2 - a''\xi\alpha + a\xi\alpha'_u + a\eta\alpha'_v = 0 \tag{2.58}$$

such that $\tilde{X}_2(V) = 0$. The transformation (2.57) reduces $\tilde{X}_2(V)$ to its canonical form

$$\tilde{Y}_2 = exp\left(\int \frac{dU}{U - V}\partial/\partial U\right) \tag{2.59}$$

and (2.53) simplifies to the obviously integrable form

$$\frac{dV}{dU} = \frac{F(V)}{V - U}. \tag{2.60}$$

(ii) If $X_1 = \rho(x, y)X_2$ for any function ρ, then

$$U = a(u), \qquad V = \left.\frac{\rho'}{\rho}\right|_{(u,v)} \tag{2.61}$$

where $\tilde{X}_2(a) = 0$. The transformation (2.61) reduces $\tilde{X}_2(V)$ to its canonical form

$$\tilde{Y}_2 = -V exp\left(-\int V dU\right)\partial/\partial U \tag{2.62}$$

and (2.53) simplifies to the easily integrable Bernoulli equation

$$\frac{dV}{dU} = F(U)V - V^2. \tag{2.63}$$

According to Adam and Mahomed [2, 3] the method described can also be utilized as a non-local symmetry method for the double reduction of order for second-order equations, and can be extended to higher-order equations.

2.5 First integrals of the Pohozaev-Trudinger case of a quasilinear differential equation

Bozhkov [18] was concerned with discussing a common property of certain classes of quasilinear differential equations. The property he was interested in was: *a Lie point* *symmetry of the considered equation is a Noether symmetry if and only if the equation parameters assume critical values.* Bozhkov [18] was inspired by the author Clèment et al. [24] who introduced the following equation

$$-(x^{\alpha}|y'|^{\beta}y')' = \lambda x^{\gamma} f(y) \tag{2.64}$$

where $' = d/dx$, α, β and γ are real, $x > 0$, $y = y(x)$ and the function f is nonnegative. Equation (2.64) is considered for $x \in (0, R)$, $0 < R \leq \infty$, with the conditions

$$y'(0) = 0, \qquad y(R) = 0 \tag{2.65}$$

and one looks for positive solutions. According to [24] we have two cases to distinguish between:

- The Sobolev case: $f(y) = \lambda y^p$, $\lambda = \mathit{constant}$ and $\alpha - \beta - 1 > 0$
- The Pohozaev-Trudinger case: $f(y) = \lambda e^y$, $\lambda = \mathit{constant}$ and $\alpha = \beta + 1$

Since we are considering the Lane-Emden equation of the second-kind we will consider the Pohozaev-Trudinger case in the following Section.

2.5.1 The Pohozaev-Trudinger case

When we assume that for equation (2.64)

$$\alpha - \beta - 1 = 0, \qquad \beta > -1, \qquad \gamma > -1 \tag{2.66}$$

with $f(y) = e^y$ then the situation corresponds to the Pohozaev-Trudinger case. It can be proved that if $\lambda \leq 0$ or if λ is greater than a certain positive λ^* then there is no solution to the boundary value problem (2.64), [18]. Clèment et al. [24] found the constant λ^*, proved that there is only one solution when $\lambda = \lambda^*$, and showed that there exists exactly two solutions when $0 < \lambda < \lambda^*$. Using the method for first integrals they then found explicit formulas for these solutions. The success of this approach relies heavily on the fact that $\alpha = \beta + 1$ holds if and only if all the Lie point symmetries are variational symmetries, which means that the order of the integration procedure reduces by two, [18].

Bozhkov [18] presents the result obtained in [24] in reduced form. He gives the Lie point symmetry group generator of (2.64) as

$$X_1 = -\frac{1}{m}x\frac{\partial}{\partial x} + \frac{\partial}{\partial y} \tag{2.67}$$

where $m = \gamma - \alpha + \beta + 2$. If $\beta = 0$ and $\alpha = 1$ then the symmetry group is the two-parameter Lie group determined by X_1 and

$$X_2 = \frac{1}{1+\gamma}(\frac{2}{1+\gamma}x - x\ln x)\frac{\partial}{\partial x} + \ln x\frac{\partial}{\partial y}. \tag{2.68}$$

These generators are found in subsequent Chapters through the application of Lie group theory [13, 44] in order to obtain first integrals that may be used to obtain solutions to the relevant equations. Bozhkov [18] further examines the conclusions drawn above to discover that for $\beta = 0$ and $\alpha = 1$ the Lie point symmetry group is two-dimensional. From this Bozhkov [18] deduces that there exists a one-dimensional subgroup consisting of variational symmetries. The following first integral is obtained

$$\psi(x, y, y') = \alpha x^{\alpha+1}|y'|^{\alpha+1} - (\alpha + 1)(\gamma + 1)x^{\alpha}|y'|^{\alpha} + \lambda(\alpha + 1)x^{\gamma+1}e^{y} = 0 \tag{2.69}$$

which coincides with the first integral attained in [24]. Bozhkov [18] then expresses y in terms of x and y' using (2.69) and substitutes this into equation (2.64) where $f(y) = e^y$. The following Bernoulli equation was obtained

$$y'' = \frac{\gamma - \alpha + 1}{\alpha}\frac{1}{x}y' + \frac{1}{\alpha+1}y'^2 \tag{2.70}$$

which can easily be solved to find the solution

$$y(x) = -(\alpha + 1)\ln|c_1 - \frac{\alpha}{(\alpha+1)(\gamma+1)}x^{\frac{(\gamma+1)}{\alpha}}| + c_2. \tag{2.71}$$

Some of the solutions found in this thesis maintain the form of the solution given above; it is also the case for certain first integrals obtained. Specifically if we use the values $\lambda = 1$, $\beta = 0$ and $\alpha = \gamma$ we obtain the Lane-Emden equation of the second-kind (2.28), where the parameter α becomes the shape factor.

Chapter 3

Approximate implicit solution of a Lane-Emden equation with shape factor two

The work in this Chapter has appeared in:

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In this Chapter of the thesis we consider the Lane-Emden equation of the second-kind as a model for the dimensionless density distribution in an isothermal gas sphere. We use the Lie group method to reduce the equation under consideration to a first-order ordinary differential equation. As we are unable to determine an analytical solution admitted by the reduced equation, we obtain a power series solution. This transforms into an approximate implicit solution of the original equation. The new approximate implicit solution has a larger radius of convergence than the power series solution. The approximate implicit solution diverges away from the power series solution in the radius of convergence.

3.1 Introduction

A Lane-Emden equation of the second-kind, as derived in Chapter 2, is able to describe the dimensionless density distribution in an isothermal gas sphere. The parameter value of the shape factor, k, required for this type of model is two since the density distribution occurs within a sphere. With reference to equation (2.28), derived in Chapter 2, we consider the Frank-Kamenetskii parameter [29], δ, to be one under these circumstances. The equation

$$y'' + \frac{2}{x}y' + e^{y} = 0 \tag{3.1}$$

where $' = d/dx$, describes the non-dimensional density distribution, y, in an isothermal gas sphere. Equation (3.1) is solved subject to the initial conditions

$$y(0) = y'(0) = 0. \tag{3.2}$$

The boundary condition maintaining a central density of zero is consistent with the substitution used in Chapter 2, $\rho = \rho_c e^{-y}$. Using the condition $y(0) = 0$ we find that $\rho = \rho_c e^{-y(0)} = \rho_c$ which is consistent with our definition of ρ_c as the density at the center of the star.

A second-order nonlinear ordinary differential equation derived by Bonnor [15] can be obtained by making the transformation

$$y \to -y. \tag{3.3}$$

In this way we are able to transform equation (3.1) into an equation

$$y'' + \frac{2}{x}y' - e^{-y} = 0 \tag{3.4}$$

capable of describing what is now commonly known as Bonnor-Ebert gas spheres. The transformation

$$x \to \imath x, \qquad y \to -y \tag{3.5}$$

is used to transform equation(3.1) into

$$y'' + \frac{2}{x}y' + e^{-y} = 0 \tag{3.6}$$

where (3.6) is solved subject to the initial conditions (3.2). This equation (3.6) is used in Richardson's theory of thermionic currents [58] which is related to the emission of electricity from hot bodies.

Work done by Chandrasekhar [22], Wazwaz [67], Nouh [54] and Liu [49] lead to the attainment of power series solutions admitted by the Lane-Emden equation when it models the dimensionless density distribution in a sphere. In this Chapter we are interested in obtaining an approximate implicit solution for equation (3.1). We will also attain a larger radius of convergence for our new solution than the power series solution admitted by (3.1).

3.2 Power series solution

Power series solutions are considered to be good solutions, since they give reasonable approximations to the solution on a small domain. Convergence tends to be trivial to prove and it is relatively easy to use the power series solution to analyze the behavior of equation (3.1). It can easily be shown that the second-order ordinary differential equation (3.1) admits a power series solution of the form

$$y(x) = \sum_{n=0}^{\infty} b_n x^n \tag{3.7}$$

where

$$b_0 = b_1 = 0, \tag{3.8}$$

$$b_2 = -\frac{1}{6}, \tag{3.9}$$

$$b_n = \frac{1}{2n + n(n-1)} \sum_{m=0}^{\infty} \frac{P_{m,n-2}}{m!} \tag{3.10}$$

and

$$P_{m,n} = \sum_{k_m=0}^{n} b_{n-k_m} P_{m-1,k_m}. \tag{3.11}$$

The formula (3.10) yields

$$b_n = 0, \qquad n = 3, 5, 7, 9, \ldots. \tag{3.12}$$

The term $P_{m,n}$ is defined as a recursive formula. Some of the coefficient values through the use of this formula are given by

$$\begin{aligned} b_4 &= -\frac{1}{20}b_2, \\ b_6 &= -\frac{1}{84}((b_2)^2 + 2b_4), \\ b_8 &= -\frac{1}{432}((b_2)^3 + 6b_2b_4 + 6b_6), \\ b_{10} &= -\frac{1}{2640}((b_2)^4 + 12(b_2)^2b_4 + 12(b_4)^2 + 24b_2b_6 + 24b_8), \cdots \end{aligned} \tag{3.13}$$

In fact, the power series solution (3.7) admitted by (3.1) is exactly the Adomian decomposition solution obtained by Wazwaz [67]. We note that since he obtained this solution through Adomian decomposition it is guaranteed to converge, [67].

The values given above (3.13) indicate that the coefficients b_n of the power series solution (3.7) form an even alternating sequence. We use the ratio test where we consider only the non-zero even terms of the coefficients b_n as follows

$$\begin{aligned} &\lim_{n\to\infty}\left|\frac{b_{2n+2}x^{2n+2}}{b_{2n}x^{2n}}\right| \\ &= x^2 \lim_{n\to\infty}\left|\frac{b_{2n+2}}{b_{2n}}\right|. \end{aligned} \tag{3.14}$$

Considering the numerical values of the coefficients in the following fashion

$$\left|\frac{b_4}{b_2}\right| < \left|\frac{b_6}{b_4}\right| < \left|\frac{b_8}{b_6}\right| < \cdots < \left|\frac{b_{j+2}}{b_j}\right| < \cdots \tag{3.15}$$

we find that

$$\left|\frac{b_4}{b_2}\right| = 0.05, \left|\frac{b_6}{b_4}\right| = 0.0634921, \left|\frac{b_8}{b_6}\right| = 0.0706019, \left|\frac{b_{10}}{b_8}\right| = 0.0749925. \tag{3.16}$$

From (3.16) we note that the fractions are below one but that they do increase. For convergence of the power series we require that the limit (3.14) be less than one. Hence for the power series to converge we require that $|x^2| < 1$. From this we determine that the power series (3.7) converges on the domain given by

$$|x| < 1 \tag{3.17}$$

since the series is even, [41, 57].

When $x = 1$ we find that the power series solution (3.7) simplifies to

$$y(1) = \sum_{n=0}^{\infty} b_n. \tag{3.18}$$

Since the power series solution (3.7) is alternating and decreasing we have that

$$y(1) < -\frac{1}{6}. \tag{3.19}$$

Therefore, from (2.6) for the power series solution (3.7) admitted by (3.1) we find that

$$\frac{\rho}{\rho_c} > 1.18136. \tag{3.20}$$

Therefore, we have that the power series solution is valid on the dimensional domain

$$r < \left[\frac{K}{4\pi G\rho_c}\right]^{1/2} \tag{3.21}$$

with constants as defined in Chapter 2.

3.3 Lie Group Reduction

In order to reduce the order of equation (3.1) we apply the Lie group method as discussed in Chapter 2, [13, 44]. We need to find the coefficients ξ and η of the infinitesimal generator (2.35). In order to do this we solve the determining equation

$$X^{[2]}F(x, y, y', y'')\big|_{y''=-(2/x)y'-e^{y}} = 0 \tag{3.22}$$

as shown in Chapter 2. The resulting system of equations can easily be solved to give

$$\xi = x, \qquad \eta = -2. \tag{3.23}$$

Therefore the infinitesimal generator admitted by (3.1) is given by

$$X = x\frac{\partial}{\partial_x} - 2\frac{\partial}{\partial_y}. \tag{3.24}$$

We then find the group invariant solution $y = \Phi(x)$ admitted by (3.1) corresponding to Lie point symmetry generator (3.24) calculated by solving the first-order ordinary differential equation obtained from Ibragimov [44]

$$X\left(y - \Phi(x)\right)\big|_{y=\Phi(x)} = 0. \tag{3.25}$$

Substituting (3.24) into (3.25) we obtain

$$x\frac{d\Phi}{dx} + 2 = 0. \tag{3.26}$$

Solving (3.26) we find that

$$y = \Phi(x) = c_0 - \ln x^2 \tag{3.27}$$

where c_0 is a constant of integration. Substituting (3.27) into (3.1) we determine the constant c_0 to find that

$$y = \ln\left(\frac{2}{x^2}\right). \tag{3.28}$$

This solution describes a singular isothermal sphere with infinite density at $x = 0$, [12].

Since (3.1) only admits one Lie point symmetry, we can use (3.24) to reduce (3.1) to first-order. A first prolongation (extension) of (3.24) is given by

$$X^{[1]} = x\frac{\partial}{\partial_x} - 2\frac{\partial}{\partial_y} - y'\frac{\partial}{\partial_{y'}} \tag{3.29}$$

where (3.23) is substituted into (2.38) to obtain $\zeta^{(1)}$. Differential invariants corresponding to (3.29) are given by

$$\overline{x} = x^2 e^y, \qquad \overline{y} = y' e^{-y/2}. \tag{3.30}$$

Imposing the initial conditions (3.2) on the invariants (3.30) we find that

$$\overline{y}\,(0) = 0. \tag{3.31}$$

We reduce the order of (3.1) by writing it in terms of the invariants (3.30) to obtain

$$\left(2\overline{x} + \overline{y}\,\overline{x}^{\,3/2}\right)\frac{d\overline{y}}{d\overline{x}} = -\left(\frac{1}{2}\overline{y}^2\,\overline{x}^{\,1/2} + 2\overline{y} + \overline{x}^{1/2}\right) \tag{3.32}$$

which can be rewritten as

$$\overline{x}\left(\overline{y} + 2\overline{x}^{\,-1/2}\right)\frac{d\overline{y}}{d\overline{x}} = -\frac{1}{2}\left[\left(\overline{y} + 2\overline{x}^{\,-1/2}\right)^2 - 4\overline{x}^{\,-1} + 2\right]. \tag{3.33}$$

We can reduce (3.33) to an Abel equation of the second-kind by making the transformation

$$\overline{\overline{y}} = \overline{x}^{1/2}\overline{y} + 2 \tag{3.34}$$

to obtain

$$\frac{1}{2}\frac{d(\overline{\overline{y}}^2)}{d\overline{x}} = -\left[1 + \frac{\overline{\overline{y}}}{\overline{x}} - \frac{2}{\overline{x}}\right]. \tag{3.35}$$

If we can find a solution

$$\overline{\overline{y}} = f\left(\overline{x}\right) \tag{3.36}$$

admitted by (3.35), then the transformations (3.34) and (3.30) imply that $y(x)$ must satisfy the first-order ordinary differential equation

$$x\frac{dy}{dx} = f(x^2 e^y) - 2. \tag{3.37}$$

The initial conditions (3.2) then become

$$\overline{\overline{y}}(0) = 2. \tag{3.38}$$

The first-order ordinary differential equation (3.35) is not in the class of ordinary differential equations considered by Abraham-Shrauner and Guo [1] and Adam and Mahomed [2, 3] nor is a solution to be found in the handbook by Polyanin and Zaitsev [56]. It is singular when $\overline{x} = 0$ and/or $\overline{\overline{y}} = 0$.

3.4 Approximate implicit solution

It can be shown that the first-order ordinary differential equation (3.35) admits the power series solution

$$\overline{\overline{y}} = \sum_{n=0}^{\infty} a_n \overline{x}^n \tag{3.39}$$

$$a_0 = 2, \qquad a_1 = \frac{1}{3} \tag{3.40}$$

$$a_n = -\left(\frac{n}{2+4n}\right)\sum_{k=1}^{n-1} a_k a_{n-k}. \tag{3.41}$$

The power series solution (3.39) satisfies the initial condition $\overline{\overline{y}}(0) = 2$. We note that the coefficients of the power series (3.39) form an alternating sequence for $n \geq 1$. Using the ratio test we find that the power series solution (3.39) admitted by (3.35) converges absolutely for $\overline{x} \in \mathbb{R}$ on the domain $|\overline{x}| < 1$. We discover this by considering the ratio test as follows

$$\begin{aligned} &\lim_{n\to\infty}\left|\frac{a_{n+1}\overline{x}^{n+1}}{a_n\overline{x}^n}\right| \\ &= \overline{x}\lim_{n\to\infty}\left|\frac{a_{n+1}}{a_n}\right|. \end{aligned} \tag{3.42}$$

We assess the coefficients a_n and realise that the series of inequalities (3.15) is similarly maintained by the coefficients. In fact we find that

$$\left|\frac{a_2}{a_1}\right| = 0.0666667, \left|\frac{a_3}{a_2}\right| = 0.142857, \left|\frac{a_4}{a_3}\right| = 0.182716, \left|\frac{a_5}{a_4}\right| = 0.206798, \left|\frac{a_6}{a_5}\right| = 0.222831. \tag{3.43}$$

Since the terms $|\frac{a_{n+1}}{a_n}|$ are increasing to maintain convergence for the power series (3.7) by attaining a limit (3.42) of less than one, as per the ratio test, we must maintain that $|\overline{x}| < 1$. Hence the power series solution (3.39) admitted by (3.35) converges absolutely for $\overline{x} \in \mathbb{R}$ on the domain $|\overline{x}| < 1$, [41, 57].

From (3.30) condition $|\overline{x}| < 1$ implies that the group invariant solution is only valid on the domain

$$|x^2 e^y| < 1. \tag{3.44}$$

If we let

$$y^* = \ln x^2 e^y \tag{3.45}$$

then (3.37) simplifies to the separable form

$$\frac{dy^*}{dx} = \frac{f(e^{y^*})}{x} \tag{3.46}$$

where

$$f(\overline{x}) = \sum_{n=0}^{\infty} a_n \overline{x}^n. \tag{3.47}$$

We now determine an approximate solution to (3.46) using a finite number of terms in the power series solution (3.39). The first-order ordinary differential equation (3.46) can be integrated once to obtain

$$\ln x + k = \int \left[\sum_{n=0}^{\infty} a_n e^{ny^*} \right]^{-1} dy^* \tag{3.48}$$

where k is a constant of integration. We can write the integral in (3.48) as

$$\int a_0^{-1} \left[1 + \sum_{n=1}^{\infty} \frac{a_n}{a_0} e^{ny^*} \right]^{-1} dy^*. \tag{3.49}$$

We can obtain an approximate solution to (3.48) by writing the infinite sum in (3.49) as a finite sum to obtain

$$\ln x + k = \int a_0^{-1} \left[1 + \sum_{n=1}^{m} \frac{a_n}{a_0} e^{ny^*} \right]^{-1} dy^*. \tag{3.50}$$

From the definition of the constants a_i given by (3.40) and (3.41) we can prove that the partial sum S_m where

$$S_m = \sum_{n=1}^{m} \frac{a_n}{a_0} e^{ny^*} = \frac{a_1}{a_0} e^{y^*} + \frac{a_2}{a_0} e^{2y^*} + \ldots + \frac{a_m}{a_0} e^{my^*} \tag{3.51}$$

is bounded above by one, i.e.

$$S_m < 1. \tag{3.52}$$

As a consequence of this condition (3.52) we use the approximation $(1+x)^n = 1 + nx + n(n-1)x^2 + \cdots$ so that we may rewrite (3.50) as follows

$$\ln x + k = \int a_0^{-1} \left[1 - \sum_{n=1}^{m} \frac{a_n}{a_0} e^{ny^*} \right] dy^*. \tag{3.53}$$

Since $S_m < 1$ the terms $(S_m)^2, (S_m)^3, (S_m)^4, \cdots$ are small enough so that we assume them to be negligible. Equation (3.53) can be integrated to obtain

$$\ln x + k = \frac{y^*}{a_0} - \sum_{n=1}^{m} \frac{a_n}{n a_0^2} e^{ny^*}. \tag{3.54}$$

Substituting (3.45) into (3.54) and simplifying we find that

$$2k = y - \sum_{n=1}^{m} \frac{a_n}{2n} x^{2n} e^{ny}. \tag{3.55}$$

Imposing the initial condition $y(0) = 0$ from (3.2) we find that

$$y = \sum_{n=1}^{m} \frac{a_n}{2n} x^{2n} e^{ny}. \tag{3.56}$$

Equation (3.56) is a new approximate implicit solution admitted by (3.1) valid on the domain (3.44). Imposing (3.3) on (3.56) we obtain

$$y = -\sum_{n=1}^{m} \frac{a_n}{2n} x^{2n} e^{-ny} \tag{3.57}$$

which is a new approximate implicit solution admitted by (3.4) for Bonnor-Ebert spheres, [15]. Imposing (3.5) on the solution (3.56) we obtain

$$y = -\sum_{n=1}^{m} \frac{a_n}{2n} (-1)^n x^{2n} e^{-ny} \tag{3.58}$$

which is a solution admitted by (3.6) for Richardson's theory of thermionic currents, [58].

From condition (3.44) we find that

$$y < \ln\left(\frac{1}{x^2}\right). \tag{3.59}$$

Using this condition with the transformations (2.6) given in Chapter 2

$$\rho = \rho_c e^{-y}, \qquad r = \left[\frac{K}{4\pi G \rho_c}\right]^{1/2} x \tag{3.60}$$

we find that

$$\frac{\rho}{\rho_c} > x^2 \tag{3.61}$$

where ρ is defined as the spatial density and ρ_c as the central density. From the transformation (3.3) for a Bonnor-Ebert sphere we have that

$$\frac{\rho}{\rho_c} < \frac{1}{x^2}. \tag{3.62}$$

Substituting $y = \ln(1/x^2)$ into (3.56) and solving we find that

$$x = \exp\left(-\sum_{n=1}^{m} \frac{a_n}{4n}\right) \tag{3.63}$$

which indicates that we have obtained a larger radius of convergence that the straightforward power series solution (3.7).

We can use the generator of infinitesimal transformations (3.24) to transform the power series solution (3.7) and approximate implicit solution (3.39) into new solutions admitted by (3.1). Using the coefficients of (3.24) we solve the system of first-order ordinary differential equations

$$\frac{dx^*}{da} = x, \qquad \frac{dy^*}{da} = -2 \tag{3.64}$$

where a is the group parameter. The system (3.64) is solved subject to the initial conditions $x^*(0) = x$ and $y^*(0) = y$ to find that

$$x^* = e^a x, \qquad y^* = y - 2a. \tag{3.65}$$

The invariant solution (3.28) is maintained under the transformations (3.65). Non-invariant solutions of the form $y = f(x)$ like (3.7) and (3.39) are transformed into the solution

$$y^* = f(e^{-a}x^*) - 2a \tag{3.66}$$

admitted by (3.1). The initial conditions (3.2) transform into

$$x^* = 0, \qquad y^* = -2a, \qquad \frac{dy^*}{dx^*} = 0. \tag{3.67}$$

Therefore the invariant solutions will not satisfy the initial condition $y(0) = 0$. This implies that transformations of any non-invariant solution $y = f(x)$ admitted by (3.1) given by (3.66) will satisfy $y'(0) = 0 = dy^*(0)/dx^*$ but not the initial condition $y(0) = 0 \neq y^*(0) = -2a$. This leads to a much wider class of solutions that satisfy only the derivative initial boundary condition from (3.2).

3.5 Numerical comparison of results

In the above Section we claim that it can be shown that the first-order ordinary differential equation (3.35) admits the power series solution (3.39). Some of the terms of this solution, defined above by equation (3.41), are given by

Table 3.1: *Ratios required for the stability analysis of the isothermal gas sphere.*

m	x	x^2	$\ln(1/x^2)$
1	1.08690404952123	1.18136041286565	-0.16666666666667
2	1.08992742462461	1.18794179094884	-0.17222222222222
3	1.09021580335679	1.18857049788889	-0.17275132275132
4	1.09025532786779	1.18865667994409	-0.17282382912013
5	1.09026186686851	1.18867093834761	-0.17283582444076
10	1.09026339081407	1.18867426134940	-0.17283861999758

$$\begin{aligned} a_0 &= 2, \\ a_1 &= -\tfrac{1}{3}, \\ a_2 &= -\tfrac{1}{45}, \\ a_3 &= -\tfrac{1}{315}, \\ a_4 &= -\tfrac{74}{127575}, \\ a_5 &= -\tfrac{101}{841995}, \\ \vdots & \quad \vdots \quad \vdots \end{aligned} \tag{3.68}$$

Using the values obtained for these coefficients we are able to use equation (3.63) to obtain a table of values to assess the stability of the isothermal sphere under consideration. These ratio's are computed for different values of m and displayed in Table 3.1.

From the values attained in Table 3.1 we find that for $m = 10$ the ratio (3.61) becomes

$$\frac{\rho}{\rho_c} > 1.18867426134940. \tag{3.69}$$

The ratio given in (3.69) is larger than the limit given in (3.20) by 0.00731385. Also, from Table 3.1 we have that

$$x < 1.091 \tag{3.70}$$

and therefore from (3.60) we have that

$$r < 1.091 \left[\frac{K}{4\pi G \rho_c} \right]^{1/2}. \tag{3.71}$$

The solution (3.56) is computationally more expensive than computing the power series solution (3.7). By specifying x we end up having to solve a nonlinear equation. This complication is somewhat simplified if we consider (3.56) as a polynomial in x, where x is the value to be calculated when y is specified. A possible algorithm would read as follows: discretize the interval $y \in [0, -0.172839]$ where the boundary value 0 comes from (3.2) and -0.172839 is obtained from Table 3.1. We specify a $y = y_p$ value from the interval. We then have to solve the following polynomial equation for $x = x_p$:

$$\sum_{n=1}^{m} \frac{a_n}{2n} {x_p}^{2n} e^{ny_p} - y_p = 0. \tag{3.72}$$

Expanding (3.72) we find that

$$\frac{a_1}{2} {x_p}^2 e^{y_p} + \frac{a_2}{4} {x_p}^4 e^{2y_p} + \frac{a_3}{6} {x_p}^6 e^{3y_p} + \ldots + \frac{a_m}{2m} x^{2m} e^{my_p} - y_p = 0. \tag{3.73}$$

Solving the nonlinear equation (3.73) using MATHEMATICA we obtain rapid convergence to the solution.

From Figure 3.1, where we have taken $m = 14$, we note that the radius of convergence of the approximate implicit solution (3.56) is bounded by the curve $y = \ln(1/x^2)$ while the radius of convergence of (3.57) is bounded by $y = -\ln(1/x^2)$. We are unable to determine an upper bound on (3.58) because the transformation (3.5) leaves (3.59) imaginary. The numerical solution follows the power series solution very closely. In the domain $x \in [0, 1]$ we note that the approximate implicit solution diverges from the power series solution. This deviation from the power series solution is not a numerical anomaly.

From (3.18) we have an expression for $y(1)$ for the power series solution (3.7). Writing (3.56) as follows

$$z(x) = y - \sum_{n=1}^{m} \frac{a_n}{2n} x^{2n} e^{ny} \tag{3.74}$$

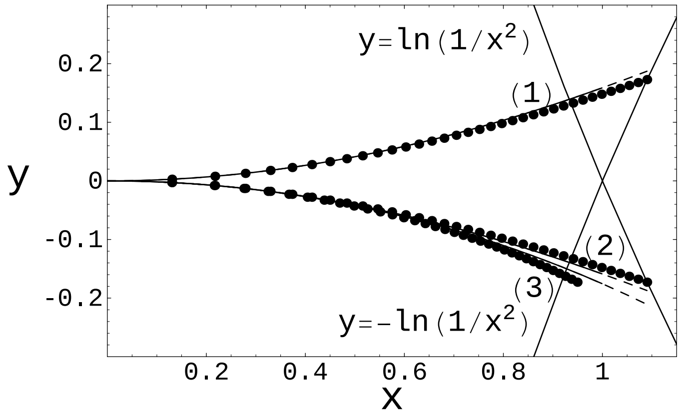

Figure 3.1: *Plot comparing the numerical solution (− − −), power series solution (____) and the new implicit solution (• • •) for* (1) *Bonnor-Ebert spheres,* (2) *equation (3.1) and* (3) *Richardson's theory of thermionic currents.*

and evaluating (3.74) at $x = 1$ we obtain

$$z(1) = y(1) - \sum_{n=1}^{m} \frac{a_n}{2n}\, e^{ny(1)}. \tag{3.75}$$

Substituting the expression for $y(1)$ from (3.18) we find that

$$z(1) = \sum_{n=0}^{\infty} b_n - \sum_{n=1}^{m} \frac{a_n}{2n}\, e^{n\sum_{n=0}^{\infty} b_n}. \tag{3.76}$$

It would be very convenient if the power series solution and the new implicit solution could tend to each other as $m \to \infty$. If this is the case then we should have that $z(1) \to 0$. If we take the limit as $n \to \infty$ it implies that $m \to \infty$ in the summation for the approximate implicit solution. Doing so we find that (3.76) becomes

$$\lim_{n\to\infty} z(1) < -\frac{1}{6} - \sum_{n=1}^{\infty} \frac{a_n}{2n} e^{-n/6} \tag{3.77}$$

where we have imposed the limiting condition (3.19). Since the coefficients a_n are negative for $n > 1$ we find that

$$\lim_{n\to\infty} z(1) > 0. \tag{3.78}$$

This proves that as $m \to \infty$ the new implicit approximate solution diverges from the power series solution. If we consider only the interval $x \in [0, 1]$ we get the difference

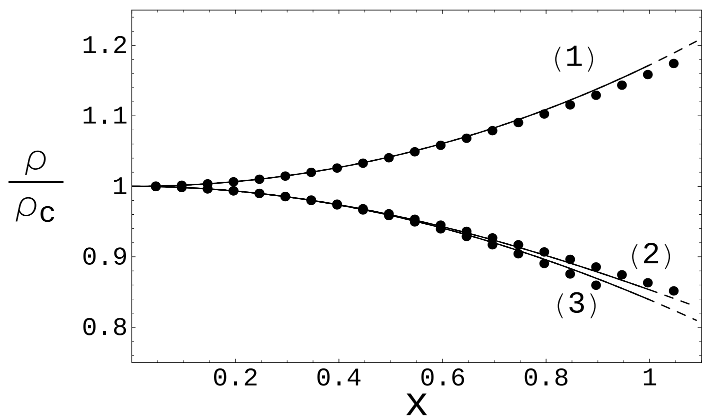

Figure 3.2: *Plot comparing the ratio ρ/ρ_c for the numerical solution (− − −), power series solution (____) and the new implicit solution (•••) for (1) Bonnor-Ebert spheres, (2) equation (3.1) and (3) Richardson's theory of thermionic currents.*

table, Table 3.2, where y is the power series solution (3.7) and y^* the approximate implicit solution (3.56) at different x-values.

Table 3.2: *Comparison of approximate implicit solution with the power series solution.*

x	$\lvert y - y^* \rvert$	$\lvert \exp(y) - \exp(y^*) \rvert$
0	0	0
0.2	0.0000219584	0.000021813
0.4	0.0003391960	0.000330396
0.6	0.0016227900	0.001531150
0.8	0.0047569100	0.004299900
1.0	0.0106022000	0.009093340

In Figure 3.2 we compare the ratio ρ/ρ_c from (3.60). We note that the there is very little difference between the power series solution, implicit approximate solution and numerical solution. This is verified by the data given in Table 3.2.

3.6 Concluding remarks

We determined a new approximate implicit solution admitted by the Lane-Emden equation (3.1) for isothermal gas spheres. This solution was then transformed into a solution for Bonnor-Ebert spheres, [15] and Richardson's theory of thermionic currents, [58]. This was done via a Lie group-theoretic approach. Obtaining an infinitesimal generator enabled us to find differential invariants which were used to reduce the order of the equation. Through an appropriate transformation we obtain an Abel equation of the second-kind which admits a power series solution. By imposing the relevant condition and converting to the original variables we obtain an approximate implicit solution to the original Lane-Emden equation.

It is computationally more expensive to determine the new approximate implicit solution. This is easily overcome by specifying y-values and solving the equation for x. The divergence of the approximate implicit solution from the power series solution is a new phenomenon. We have shown that as $m \to \infty$ the solutions do not converge. This leads us to conclude that the divergence is not a numerical phenomenon. The ratio ρ/ρ_c for both the power series solution and the approximate implicit solution does not diverge as severely. The approximate implicit solution has a larger radius of convergence than the power series solution. Hunter [41] has shown how the radius of convergence can be increased by means of an Euler transformation of the Lane-Emden equation. In this Chapter we obtained a similar result using a Lie symmetry reduction. This is useful provided the ratio ρ/ρ_c is within the limits of stability for the isothermal gas sphere under consideration, [15, 23]. Though the improvement on the radius of convergence may seem minor it is important to note that the equation under consideration is dimensionless. The true improvement to the radius of convergence should be much larger when considered on the appropriate scale.

Chapter 4

Steady state solutions for a thermal explosion in a cylindrical vessel and the Frank-Kamenetskii parameter

Some of the work in this Chapter has appeared in:

Harley, C. and Momoniat, E., *Steady state solutions for a thermal explosion in a cylindrical vessel*, Modern Physics Letters , 21, (2007), 831-842.

Some of the work in this Chapter is to appear in:

Harley, C. and Momoniat, E., *Alternate derivation of the critical value of the Frank-Kamenetskii parameter in the cylindrical geometry*, J. Nonlinear Mathematical Physics, (2008).

In this Chapter steady state solutions of a heat balance equation modelling a thermal explosion in a cylindrical vessel are obtained. The heat balance equation reduces to a Lane-Emden equation of the second-kind when steady state solutions are investigated. Analytical solutions to this Lane-Emden equation of the second-kind are obtained by implementation of the Lie group method. The classical Lie group method is used to obtain the well known solution of Frank-Kamenetskii for the temperature distribution in a cylindrical vessel. Using an extension of the classical Lie group method a non-local symmetry is obtained and a new solution describing the temperature distribution after ignition is obtained.

Noether's theorem is used to determine first integrals admitted by the equation. These first integrals exist for rectangular and cylindrical geometries. Relationships between the Frank-Kamenetskii parameter, δ, and the boundary conditions for a thermal explosion within a vessel are found. These relationships enable us to obtain the well known critical value for the Frank-Kamenetskii parameter, $\delta = 2$, without solving the second-order ordinary differential equation first.

4.1 Introduction

In this Chapter of our thesis we strive to obtain steady state solutions to the heat balance equation (2.8), derived in Chapter 2, modeling a thermal explosion in a vessel. For a thermal explosion to occur the heat generated by a chemical reaction in a vessel is far greater than the heat lost to the walls of the vessel in which the reaction is taking place. The walls of the vessel are assumed to be thermally conducting. The increase in heat increases the rate of the chemical reaction exponentially following the Arrhenius equation until a thermal explosion occurs.

Under steady state conditions [29] the heat balance equation (2.8) for ignition in a vessel reduces to

$$y'' + \frac{k}{x}y' + e^y = 0 \tag{4.1}$$

where $' = d/dx$, describing the thermal explosion within a vessel. A lot of the work done in this Chapter places particular emphasis on the model of a thermal explosion occurring in a cylindrical vessel modelled by

$$y'' + \frac{1}{x}y' + e^y = 0. \tag{4.2}$$

Boundary conditions for the thermal explosion problem in a rectangular geometry, with shape factor $k = 0$, are given by [29]

$$y(\pm 1) = 0. \tag{4.3}$$

The boundary condition (4.3) fixes the temperature at the walls. Boundary conditions for the thermal explosion problem in a cylindrical geometry are given by [29]

$$y'(0) = 0, \qquad y\,(R) = -\theta_0. \tag{4.4}$$

where $R = \left[\delta e^{\theta_0}\right]^{1/2}$ with $\delta = \frac{\sigma QAE}{kRT_0^2} e^{\left(-\frac{E}{RT_0}\right)}$. These boundary conditions ensure continuity at the centre of the vessel and fix the non-dimensional temperature at the wall. If it can be shown that the temperature gradient at the boundaries $x = -1$ and $x = 1$ for the rectangular geometry are equal then the boundary condition ensuring continuity at the centre of the vessel (4.4) can be applied to (4.1) for $k = 0$.

We use the theory of Lie, [55, 13, 43], to determine differential invariants that reduce equation (4.2) for $k = 1$ to first-order. A new parametric solution admitted by the reduced first-order equation is obtained. This solution is not physical in terms of the model considered here. Further solutions of the reduced first-order equation are obtained by using the direct method of Adam and Mahomed [2, 3] to determine a non-local symmetry admitted by the reduced equation. This solution describes the ignition phenomenon within a cylindrical vessel.

Via Noether's theorem the first integrals are obtained for a rectangular and cylindrical geometry. These first integrals show the symmetry of the temperature gradients at the rectangular walls. For a cylindrical geometry the first integrals show the dependence of the critical parameter on the temperature gradient at the cylinder wall. In this way we have discovered new boundary conditions that are dependent on the parameter δ.

4.2 Reductions of order

For the thermal explosion problem within a cylindrical vessel Frank-Kamenetskii [29, 56] uses the transformations

$$p = \log x, \qquad w = y + 2\log x \tag{4.5}$$

to transform (4.2) into the autonomous second-order ordinary differential equation

$$\frac{d^2w}{dp^2} + e^w = 0. \tag{4.6}$$

Solving (4.6) we find that

$$w = \log\left[\frac{1}{2}\left(c_2 - c_2\tanh^2\left[\frac{1}{2}\sqrt{c_2}(p + c_1)\right]\right)\right] \tag{4.7}$$

where c_1 and c_2 are constants of integration. Substituting (4.5) into (4.7) we find that

$$y = \log\left[\frac{\left(c_2 - c_2\tanh^2\left[\frac{1}{2}\sqrt{c_2}(\log x + c_1)\right]\right)}{2x^2}\right]. \tag{4.8}$$

Imposing boundary conditions (4.4) Frank-Kamenetskii [29] obtains the critical values associated with the ignition transition from steady state

$$\delta = 2, \qquad \theta_0 = \log 4 \tag{4.9}$$

to obtain the solution

$$y = \log\left[\frac{64}{(8 + x^2)^2}\right]. \tag{4.10}$$

It is important to note that though the parameter δ is not explicitly observable in the equation (4.2) through the transformations (2.19) in Chapter 2 the parameter is incorporated into the boundary conditions (4.4) where $R = \left[\delta e^{\theta_0}\right]^{1/2}$. As discussed in Chapter 2, [29, 9], there is no steady state solution after combustion, i.e. where $\delta > 2$.

Chambré [21] reduces equation (4.2) to first-order by using the differential invariants [25, 16]

$$v_1 = x^2 e^y, \qquad v_2 = xy'. \tag{4.11}$$

The invariants (4.11) reduce equation (4.2) to the first-order ordinary differential equation

$$\frac{dv_2}{dv_1} = -\frac{1}{(v_2 + 2)} \tag{4.12}$$

which is easily solved to give

$$(v_2 + 2)^2 = c_3 - 2v_1 \tag{4.13}$$

where c_3 is a constant of integration. In terms of the invariants (4.11) the boundary condition used to maintain symmetry within the vessel (4.4) is written as $v_2(0) = 0$ giving $c_3 = 4$. The solution (4.13) is then written in terms of the original variables and the resulting ordinary differential equation is solved. The critical values (4.9) and solution (4.10) are again obtained.

4.2.1 Lie group analysis

Bozkhov and Martins [16] have shown that for $k = 0$ the model equation (2.28) admits the infinitesimal generators

$$Z = \frac{\partial}{\partial_x}, \qquad X = x\frac{\partial}{\partial_x} - 2\frac{\partial}{\partial_y}. \tag{4.14}$$

For the case $k = 1$ it admits the infinitesimal generator X and

$$Y = x(\log x - 1)\frac{\partial}{\partial_x} - 2\log x\frac{\partial}{\partial_y}. \tag{4.15}$$

For values of $k \neq 0, 1$ the model equation (2.28) only admits X as an infinitesimal generator. Bozkhov and Martins [16] show that X is in fact a Noether symmetry of this equation for $k = 1$. Hence for a shape factor of $k = 1$ we can apply the infinitesimal generator X coupled with Noether's theorem [53] to determine a first integral admitted by equation (4.1).

In order to obtain new solutions we consider differential invariants corresponding to a first-order extension of (4.15). These differential invariants are given by

$$v_1 = y + 2\left(\log x + \log\left(\log x - 1\right)\right), \tag{4.16}$$

$$v_2 = x\,(\log x - 1)\,y' + 2\log x. \tag{4.17}$$

The invariants (4.16) and (4.17) reduce (4.2) to the first-order ordinary differential equation

$$v_2 \frac{dv_2}{dv_1} - v_2 + e^{v_1} + 2 = 0. \tag{4.18}$$

From Polyanin and Zaitsev [56] equation (4.18) admits the parametric solution

$$v_1(t) = -2\log\left[\frac{\sqrt{2+\tau^2}}{c_4 - 2\log\left[\tau + \sqrt{2+\tau^2}\right]}\right] \tag{4.19}$$

$$v_2(t) = 2 + \frac{2}{\sqrt{2+\tau^2}}\left(c_4 - 2\log\left[\tau + \sqrt{2+\tau^2}\right]\right) \tag{4.20}$$

where c_4 is a constant. Substituting (4.19) and (4.20) into (4.16) and (4.17) we find that

$$x(\tau) = e^{1+c_4 e^{c_4}}\left(\tau + \sqrt{2+\tau^2}\right)^{-2e^{c_4}}, \tag{4.21}$$

$$y(\tau) = -\log\left[2+\tau^2\right] - 2\left(1 + c_4 + e^{c_4}\left(c_4 - 2\log\left[\tau + \sqrt{2+\tau^2}\right]\right)\right). \tag{4.22}$$

The parametric solution (4.21) and (4.22) admits only one constant of integration. The parametric solution (4.21) and (4.22) is a new solution to (4.2). By fixing the temperature at the wall of the vessel (4.4) we find that

$$\tau = -1.55598, \qquad c_4 = -1.08977 \tag{4.23}$$

where the values of (4.9) hold. We note that the boundary condition which fixes the temperature at the wall of the vessel (4.4), $x = R$, is satisfied by the choice of c_4. However the solution slope is singular at $x = 0$ corresponding to $\tau = -1.55598$ so that the symmetry condition (4.4) cannot be satisfied.

4.2.2 Non-local symmetry

In order to find an additional solution to (4.18) we consider a non-local symmetry admitted by (4.18). The transformations [2, 3]

$$u = \overline{y}, \qquad v = \overline{y}' \tag{4.24}$$

transform (4.18) into the second-order ordinary differential equation

$$\frac{d^2\overline{y}}{dx^2} - \frac{d\overline{y}}{dx} + e^{\overline{y}} + 2 = 0. \tag{4.25}$$

The second-order ordinary differential equation (4.25) admits two generators of infinitesimal transformations

$$Y_1 = -\frac{\partial}{\partial_x}, \qquad Y_2 = e^{-x}\frac{\partial}{\partial_x} + 2e^{-x}\frac{\partial}{\partial_{\overline{y}}} \tag{4.26}$$

where the commutator (Lie bracket) of operators (4.26) is given by

$$[Y_1, Y_2] = Y_2. \tag{4.27}$$

The symmetry generator Y_2 then becomes an exponential non-local symmetry generator of (4.18) given by

$$\tilde{Y_2} = \exp\left(-\int \frac{du}{v}\right)\left(2\frac{\partial}{\partial_u} + (v-2)\frac{\partial}{\partial_v}\right) \tag{4.28}$$

as shown by Adam and Mahomed [2, 3]. Using (4.28) and following the algorithm presented by Adam and Mahomed [2, 3] for the case $Y_1 \neq \rho(x,y)Y_2$ we obtain the variables

$$U = e^{u/2}, \qquad V = \frac{2e^{u/2}}{2-v}. \tag{4.29}$$

The first-order ordinary differential equation (4.18) is written in terms of the new variables (4.29) to obtain the separable first-order ordinary differential equation

$$\frac{dV}{dU} = \frac{2V + V^3}{2U - 2V}. \tag{4.30}$$

By inverting, equation (4.30) may be written as

$$\frac{dU}{dV} - \frac{2U}{2V + V^3} = \frac{-2V}{2V + V^3}. \tag{4.31}$$

which gives the integrating factor

$$If = \int \frac{-2}{2V + V^3} dV. \tag{4.32}$$

From here we are able to solve (4.30) to obtain

$$U = \frac{V}{\sqrt{2 + V^2}}\left(c_5 + \sqrt{2}\log\left[\frac{2 + \sqrt{2}\sqrt{2 + V^2}}{V}\right]\right) \tag{4.33}$$

where c_5 is a constant of integration. Substituting (4.29) into (4.33) and simplifying we find that

$$\sqrt{4e^u + 2(2-v)^2} =$$
$$2\left(c_5 + \sqrt{2}\log\left[\frac{1}{2}e^{-u/2}\left(\sqrt{2}\sqrt{4e^u + 2(2-v)^2} + 2(2-v)\right)\right]\right). \qquad (4.34)$$

The nonlinear equation (4.34) admits the solution

$$v = 2 \pm \imath\sqrt{2}e^{u/2}, \qquad c_5 = -\sqrt{2}\log\left[\mp\imath\sqrt{2}\right] \qquad (4.35)$$

where $\imath^2 = -1$. Substituting (4.16) and (4.17) into (4.35) we obtain the first-order ordinary differential equation

$$xy' \pm \imath\sqrt{2}xe^{y/2} + 2 = 0 \qquad (4.36)$$

that is solved to give

$$y = \log\left[-\frac{8}{x^2\left(c_6 + \log x^2\right)^2}\right] \qquad (4.37)$$

where c_6 is a constant of integration. The solution (4.37) is imaginary. Fixing the temperature at the wall of the vessel (4.4) and using the values given by (4.9) we find that

$$c_6 = \pm 2\imath - \log 8. \qquad (4.38)$$

The boundary condition ensuring continuity at the centre of the vessel (4.4) at $x = 0$ cannot be satisfied by this solution.

4.3 Similarity Solution

We have not investigated the phenomena of combustion that occurs within a vessel up to this point. In order to gain insight into this occurrence and solutions reflecting the point at which the thermal explosion occurs accurately we consider the following similarity solutions admitted by (2.20)

$$\frac{\partial u}{\partial t} = \frac{1}{x}\frac{\partial}{\partial x}\left(x\frac{\partial u}{\partial x}\right) + e^u. \qquad (4.39)$$

These similarity solutions have the form [68]

$$u(x,t) = h(q) - \log(T-t), \qquad q = \frac{x}{\sqrt{(T-t)}} \tag{4.40}$$

where $t = T$ is the time at which combustion occurs. For $t = T-1$ (4.40) admits the steady state solution

$$u(x,t) = y(x). \tag{4.41}$$

For $t = T+1$ (4.40) admits the steady state solution

$$u(x,t) = y(-\imath x) - \imath\pi. \tag{4.42}$$

The steady state solution (4.41) corresponds to one time step before ignition and (4.42) to one time step after ignition.

The solution (4.10) is the well known solution obtained by Frank-Kamenetskii [29] showing the steady state temperature distribution in a cylindrical vessel. In terms of the similarity solution (4.41) the steady state solution (4.10) is valid for one time step before ignition. The solution (4.37) satisfies the relationship $y(x) = y(-\imath x) - \imath\pi$. We can therefore conclude that even though the solution (4.37) is imaginary it represents a steady state solution valid for one time step after ignition. Plotting the real part of (4.37) in Figure 4.3 we observe that the solution does indeed indicate combustion at the centre of the cylinder.

To understand the significance of the imaginary solution (4.37) we write the solution (4.37) as

$$y = y_0 + \imath y_1 \tag{4.43}$$

where

$$y_0 = \log\left[\frac{8}{x^2\left(c_6 + \log x^2\right)^2}\right], \qquad y_1 = \pi \tag{4.44}$$

where we have used the fact that $\log(-1) = \imath\pi$. Substituting (4.43) into (4.2) and separating into a solution for the real and imaginary parts we obtain a system of second-order ordinary differential equations

$$y_0'' + \frac{1}{x}y_0' + e^{y_0}\cos y_1 = 0, \qquad y_1'' + \frac{1}{x}y_1' + e^{y_0}\sin y_1 = 0. \tag{4.45}$$

Setting $y_1 = \pi$ the system (4.45) reduces to

$$y_0'' + \frac{1}{x}y_0' - e^{y_0} = 0. \tag{4.46}$$

Therefore the real part of the solution (4.37) is a solution of the second-order ordinary differential equation (4.46). The second-order ordinary differential equation (4.46) transforms into (4.2) by making the transformation $x \to \pm \imath x$. This suggests that when combustion occurs there is an imaginary coordinate transformation that takes place. Future work will be concentrated on pursuing this aspect of equations capable of modelling thermal explosions.

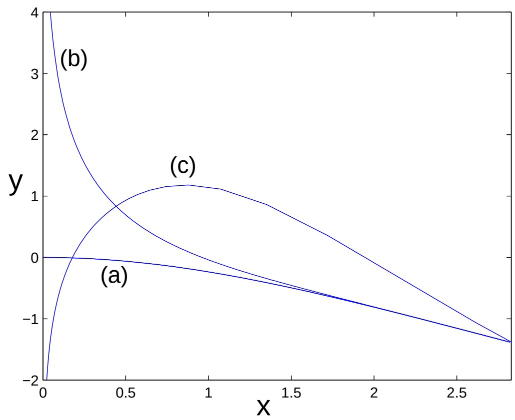

Figure 4.1: *Plot comparing (a) the solution of Frank-Kamenetskii (4.10), (b) the real part of (4.37) and (c) the parametric solution (4.21) and (4.22)*

From Figure 4.3 we note that the solution (4.10) obtained by Frank-Kamenetskii [29] and the solution (4.37) obtained from the non-local symmetry are both decreasing functions. Both solutions (4.10) and (4.37) approach the boundary $x = R$ with the same gradient. The solution (4.37) is singular at the origin. The singularity of the solution (4.37) is indicative of the phenomenon of combustion represented by this solution. The parametric solution (4.21) and (4.22) is not physical in terms of the model we are considering. The maximum height of the parametric solution (4.21) and (4.22) occurs at $x = 0.8624$ with $y = 1.1803$ and we have that as $x \to 0$, $y \to -\infty$.

4.4 Alternate derivation of the critical value δ

Finding the critical value for the Frank-Kamenetskii parameter [29] for the model equation (4.1) is most naturally done by first solving the ordinary differential equation in question. This is done by following the structure of Noether's theory [53] and finding a solution to the equation via first integrals. Through imposing the boundary conditions we find δ in terms of arbitrary constants. In maximising this function we are able to obtain the critical value of the parameter δ, i.e. the value for δ at blow-up is obtained. In this Chapter however, we look at an alternate means of finding this value.

4.4.1 Case: k = *0*

We first consider the case $k = 0$. Equation (4.1) reduces to the autonomous equation

$$y'' + \delta e^y = 0. \tag{4.47}$$

The second-order autonomous ordinary differential equation (4.47) admits the Lagrangian

$$L = y'^2 - 2\delta e^y + f(x) \tag{4.48}$$

where $f(x)$ is a gauge term. A straightforward application of (2.47) shows that Z (4.14) is a Noether symmetry of (4.48), where

$$B(x, y) = f(x). \tag{4.49}$$

From (2.50) we find that

$$I = y'^2 + 2\delta e^y. \tag{4.50}$$

It is easy to check that $D_x I = 0$ on (4.47).

Equation (4.47) admits another Lagrangian

$$L = y'^2 + y'\left(2\delta x e^y + g(y)\right) \tag{4.51}$$

with Z (4.14) as the corresponding Noether symmetry

$$B(x, y) = 2\delta e^{y} \tag{4.52}$$

the gauge term and (4.50) as the corresponding first integral.

A solution to (4.1) for $k = 0$ can be obtained by solving

$$I = \text{constant} = c_0 \tag{4.53}$$

for c_0 a constant. Substituting (4.50) into (4.53) we obtain

$$y'^2 = c_0 - 2\delta e^{y}. \tag{4.54}$$

Imposing (4.3) we find that

$$y'^2(-1) = y'^2(1). \tag{4.55}$$

This result confirms the symmetry of the boundary conditions at the boundary walls. This result allows us to then only consider half of the rectangular geometry. We can thus impose the boundary condition required to maintain continuity across the x-plane (4.4). Imposing $y'(0) = 0$ we find that (4.54) can be written as

$$y'^2 = 2\delta \left[e^{y(0)} - e^{y} \right]. \tag{4.56}$$

We can use (4.56) instead of (4.3) to solve (4.1) for $k = 0$ and we will get the same solution. Imposing the boundary condition $y(1) = 0$ we find that

$$y'^2(1) = 2\delta \left[e^{y(0)} - 1 \right]. \tag{4.57}$$

In Figure 4.2 we plot the implicit function (4.57) for $y(0)$ by specifying values of $y'(1)$. From Figure 4.2 we note that by increasing the magnitude of the temperature gradient at the wall of the rectangular vessel, the temperature at the centre of the vessel increases exponentially.

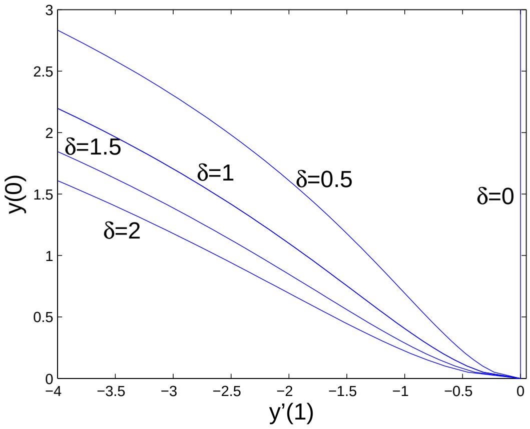

Figure 4.2: *Plot of (4.57) for different values of δ.*

4.4.2 Case: $k = 1$

For $k = 1$ Bozkhov and Martins [16] show that X from (4.14) is a Noether (variational) symmetry of the model equation (4.1). Equation (4.1) admits the Lagrangian

$$L = ax\left(\frac{1}{2}y'^2 - \delta e^y\right) + f(x) \tag{4.58}$$

where a is a constant. Using (2.50) we find the corresponding first integral

$$I = \frac{1}{2}x^2y'^2 + 2xy' + \delta x^2 e^y. \tag{4.59}$$

The approach taken by Chambré [21] is to solve the equation

$$I = c_1 \tag{4.60}$$

where c_1 is a constant. Substituting (4.59) into (4.60) and imposing $y'(0) = 0$ we obtain $c_1 = 0$. Imposing $y(1) = 0$ we find that

$$\delta = -\frac{1}{2}y'^2(1) - 2y'(1). \tag{4.61}$$

We plot the expression (4.61) in Figure 4.3. From (4.61) we find the maximal value of δ is 2, hence $y'(1) = -2$. The critical value of δ has been obtained by Frank-Kamenetskii [29] and Chambré [21] after obtaining the solution of (4.1) for $k = 1$. Here we have shown that we can determine this critical value without having to first obtain a solution to the ordinary differential equation .

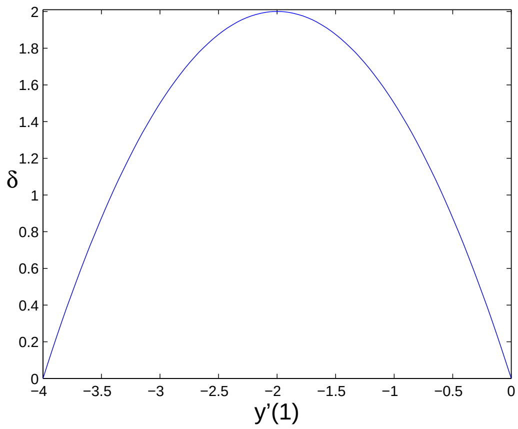

Figure 4.3: *Plot of (4.61).*

4.5 Numerical Solution

In this Section we note that the Lane-Emden equation (4.2) is singular at $x = 0$. We note that close to the origin the solution behaves like $y = a_0 - e_{a_0}\frac{x^2}{4}$ and the equation (4.2) can hence be rewritten as follows

$$y'' + \frac{1}{2}e^y = 0. \tag{4.62}$$

The solution obtained by Frank-Kamenetskii [29] (4.10) is thus far the only solution to satisfy the boundary condition at the center of the vessel. The other monotonic solution obtainable by using the approximation given is presumably physically possible however it would require an infinite flux at $x = 0$. Though solutions obtained in this way may be useful they will be unstable. We will however consider a zero flux, hence maintaining our investigation of equation (4.62).

Equation (4.62) is valid in a small interval $x \in [0, x^* \ll 1]$ about the center of the cylinder. We use `bvp4c` in MATLAB, [61], to solve (4.2) coupled with (4.62) subject to (4.4) on the interval $[0, R]$. A good guess to the solution is obtained from (4.37). We choose $x^* = 0$ in the MATLAB code. The initial guess for the derivative is taken as zero. The small increase in height at the origin is not a numerical error. By increasing the number of points in the interval $[0, R]$ we still find the height of the numerical solution at the origin is 0.1391.

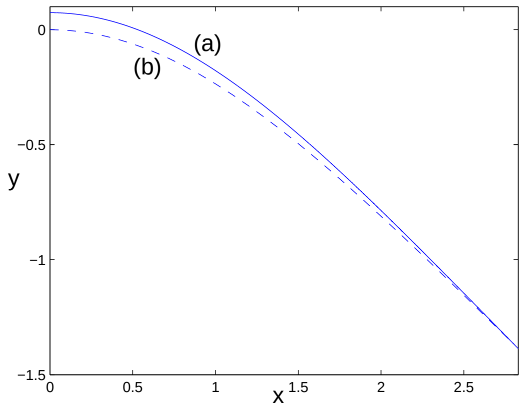

Figure 4.4: *Plot comparing (a) the numerical solution of equation (4.2) using $\widehat{bvp4c}$ in MATLAB and (b) the solution (4.10).*

Even though the change in height is small, it has implications for the activation energy when compared to the solution obtained by Frank-Kamenetskii [29]. We let the temperature at the center of the cylinder for the solution (4.10) obtained by Frank-Kamenetskii [29] be given by T_c while the temperature at the center of the cylinder for the numerical solution be given by T_n. For the numerical solution $y(0) = 0.1391$ while for the solution (4.10) $y(0) = 0$. In Chapter 2 we give Frank-Kamenetskii's [29] definition of the dimensionless temperature difference as $\theta = (E/R{T_0}^2)(T - T_0)$, where E is the energy of activation of the chemical reaction, R the universal gas constant, T the gas temperature and T_0 the temperature at the walls of the vessel. This coupled with the change of variables suggested by (2.19) in Chapter 2 gives the ratio

$$\frac{T_c - T_0}{T_n - T_0} = \frac{\theta_0}{0.1391 + \theta_0} \tag{4.63}$$

where T_0 is the temperature at the wall of the vessel. For $\theta_0 = \log 4$ the relationship (4.63) simplifies to

$$\frac{T_c - T_0}{T_n - T_0} = 0.90881. \tag{4.64}$$

Therefore the numerical solution has a higher energy increment than (4.10). A limiting condition from Frank-Kamenetskii [29] is that the temperature increment $(T - T_0)$ before the thermal explosion is of order RT_0^2/E where R is the universal gas constant and E the energy of activation. We denote the energy of activation for the solution obtained by Frank-Kamenetskii [29] as E_c and for the numerical solution E_n. Then we must have that

$$\frac{E_c}{RT_0^2}(T_c - T_0) = 1, \qquad \frac{E_n}{RT_0^2}(T_n - T_0) = 1 \tag{4.65}$$

when the activation energy is at a maximum. Therefore the ratio of the two different maximum energy activations is given by

$$\frac{E_n}{E_c} = 0.90881 \tag{4.66}$$

This shows that the maximum activation energy for the solution (4.10) obtained by Frank-Kamenetskii [29] is higher than the activation energy of the new numerical solution. The results make intuitive sense. If the activation energy of a particular chemical reaction is lower and the dimensions of the cylindrical vessel remain the same then the chemical reaction will attain a higher maximum temperature.

An alternate approach is to match the analytical solution of the linear equation (4.62) with (4.37). The analytical solution of (4.62) is given by

$$y = \log\left[c_7 - c_7 \tanh^2\left[\frac{1}{2}\sqrt{c_7}(x + c_8)\right]\right] \tag{4.67}$$

where c_7 and c_8 are constants. By ensuring continuity at the center of the vessel the constant $c_8 = 0$ in equation (4.4). Matching the solution (4.67) with the solution (4.37) at $x = x^*$ where we take $x^* = 0.1$ we find that $c_7 = 17.14704$. Therefore a solution to (4.2) can be given as

$$y = \begin{cases} \log\left[c_4 - c_4 \tanh^2\left[\frac{1}{2}\sqrt{c_4}(x + c_5)\right]\right] & 0 \leq x \leq x^* \\ \\ \log\left[-\frac{8}{x^2\left(c_3 + \log x^2\right)^2}\right] & x^* < x \leq R. \end{cases} \tag{4.68}$$

The difficulty with the solutions found above (4.68) is that they occur across different domains. Thus trying to join them over one domain will not yield a smooth solution. There are only two constants to match. The height and the initial gradient. We cannot match the gradient where the curves join. A solution of the form (4.68) gives an even higher maximum temperature with a lower activation energy.

4.6 Concluding Remarks

In this Chapter we used the Lie group method to obtain a new parametric solution as well as a singular solution using a non-local symmetry to a Lane-Emden equation of the second-kind modelling steady state solutions of a heat balance equation. The parametric solution we have obtained is not physical in terms of the model we are considering. The solution obtained from the non-local symmetry approach is a new solution describing the blow-up phenomenon.

In Section 4.4 we used first integrals obtained via Noether's theorem [53] to determine relationships between the boundary conditions of the thermal explosion problem and the critical value at which the explosion occurs, δ. For the case $k = 0$, a rectangular geometry, we have shown the symmetry of the temperature gradient at the boundary walls. We have also obtained two new boundary conditions, one of which is dependant on the value of the Frank-Kamenetskii parameter, that can be used to solve (4.1) for $k = 0$. By using this physical symmetry and imposing the boundary conditions that correspond to the cylindrical geometry case we have shown how the temperature at the centre of the rectangular vessel can be controlled by modifying the temperature gradient at the walls of the rectangular vessel. For the case $k = 1$, a cylindrical geometry, we have shown how the critical value of $\delta = 2$ can easily be obtained without recourse to a solution of the problem. These results have given us both mathematical and physical insights into the problem.

The solution obtained by Frank-Kamenetskii [29] describing combustion within a cylindrical vessel is exact. In order to investigate the behaviour of the model at the critical condition of ignition we consider certain approximations to the equation (4.2). Different approximations will increase the impact of different terms in the equation revealing different solutions of the model particularly at the point of ignition. In Section 4.5 the solution obtained using non-local symmetries is used as an initial guess in the boundary value problem solver `bvp4c` in MATLAB to obtain a new numerical solution to a linearized version of the equation (4.2). The new numerical solution has a lower activation energy and attains a higher maximum temperature at the centre of the cylinder when compared with the solution obtained by Frank-Kamenetskii [29].

The novelty of the approach taken in this Chapter is the critical condition of ignition is observed from the ordinary differential equation and not by solving a partial differential equation as is usually the case. Combustion occurring from a single point has been well studied from a partial differential equation perspective, [20, 30, 40, 51, 65, 66, 31].

Chapter 5

Instability of invariant boundary conditions of a generalised Lane-Emden equation of the second-kind

Some of the work in this Chapter has appeared in:

Harley, C. and Momoniat, E., *Instability of invariant boundary conditions of a Lane-Emden equation of the second-kind*, Applied Maths and Computation, 198, (2008), 621–633.

We use a generator of infinitesimal transformations admitted by a Lane-Emden equation of the second-kind for arbitrary shape factor k to determine invariant boundary conditions admitted by the equation. The infinitesimal generator is then used to reduce the order of the Lane-Emden equation. A phase-plane analysis of the reduced equation indicates that the stability of the invariant boundary condition $y' = 0$ on the line $x = 0$ changes with changing shape factor k. We show that for values of the shape factor $k > 1$ the boundary condition $y' = 0$ is stable on the line $x = 0$ while it is unstable for $k \leq 1$.

We also show that this instability does not manifest when solving an initial value problem. We overcome the instability by using a central difference approximation to the derivatives in our model equation. Efficient ways of calculating an initial guess to the boundary value problem in order to overcome the instability of the boundary condition $y'(0) = 0$ for $k \leq 1$ are given.

5.1 Introduction

The problem we consider in this Chapter is a boundary value problem. In an attempt to investigate the stability of the ordinary differential equation we consider in this thesis, especially with respect to the boundary conditions, we conduct a local analysis of solutions in the vicinity of what are called critical points. To do this however we first consider the invariance of the problem we aim to consider and how it may be of use to us. I tis known that if a boundary value problem is to be invariant with respect to a group G then we must also consider the invariance of the boundary (or initial) manifold [42]. We would like to determine invariant boundary conditions admitted by the equation under consideration using infinitesimal generators that leave the form invariant.

We consider the invariant boundary conditions admitted by the Lane-Emden equation of the second-kind

$$y'' + \frac{k}{x}y' + \delta e^y = 0 \tag{5.1}$$

where $' = d/dx$ and k and δ are both constants. We determine invariant boundary conditions admitted by (5.1) by imposing the infinitesimal operator that leaves (5.1) form invariant for general k on arbitrary boundary conditions. These boundary conditions are different to the boundary conditions used in very specific applications of (5.1). These new boundary conditions provide some interesting insights into the behaviour of (5.1) and the stability of the boundary conditions for numerical computation. One of the approaches used by Shampine et al. [61], collocation, is used by the program `bvp4c` in MATLAB to solve boundary value problems in this Chapter. We make use of this package to demonstrate the instability of the boundary condition $y' = 0$ on the line $x = 0$.

Boundary conditions for the thermal explosion problem are given by

$$y'(0) = 0, \qquad y(1) = 0. \tag{5.2}$$

These conditions are obtained due to dimensionless transformations [21] imposed on the steady state heat balance equation as discussed in Chapter 2. For astrophysical applications (5.1) is solved subject to the initial conditions

$$y(0) = y'(0) = 0. \tag{5.3}$$

For the case $k = 2$ equation (5.1) subject to (5.3) describes the non-dimensional density distribution in an isothermal gas sphere.

We will first proceed with the attainment of invariant boundary conditions via Lie point symmetries. The stability of these boundary conditions are then investigated through a dynamical systems analysis so that we may deduce some global behaviour of the solutions. Through considering a numerical solution we demonstrate an instability found in this way and propose ways of overcoming it. This is done by either specifying the values of the initial conditions or supplying a function as an initial guess. Analytical solutions over different domains of the shape factor are also obtained as initial guesses in an attempt to overcome the instability discovered in the boundary conditions.

5.2 Invariant boundary conditions

In order to determine invariant boundary conditions admitted by (5.1) from infinitesimal generators that leave (5.1) form invariant we make use of the following principle stated in Ibragimov [42]: *If a boundary value problem is invariant with respect to a group G then a solution of the problem should be looked for in the class of invariant functions under G. Invariance of a boundary problem for a given differential equation involves the invariance (1) of the differential equation under consideration, (2) of the* *boundary (or initial) manifold, and (3) of the data to the problem under the action of G on the boundary manifold.* In this Section this principle is applied to the ordinary differential equation (5.1).

The invariance principle discussed by Ibragimov [42] is given in terms of the following definition and theorem by Bluman and Kumei [13]: *Given a scalar boundary value problem (BVP) for a $k-th$ order partial differential equation*

$$F\left(\mathbf{x}, u, u_1, u_2, \ldots, u_k\right) = 0 \tag{5.4}$$

where u_i is the set of all i-th order derivatives of u with respect to $\mathbf{x}$ defined on a domain $\Omega_{\mathbf{x}}$ in the space $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ with boundary conditions

$$B_\alpha\left(x, u, u_1, \ldots, u_{k-1}\right) = 0 \tag{5.5}$$

prescribed on boundary surfaces

$$\omega_\alpha(\mathbf{x}) = 0 \tag{5.6}$$

for $\alpha = 1, 2, \ldots, s$. We assume the BVP (5.4)-(5.6) has a unique solution. We consider an infinitesimal generator of the form

$$X = \xi_i(\mathbf{x})\frac{\partial}{\partial x_i} + \eta(\mathbf{x}, u)\frac{\partial}{\partial u} \tag{5.7}$$

which defines a one-parameter Lie group of transformations in x-space as well as (x, u) space.

Definition 1 *X is admitted by the BVP (5.4)-(5.6) if and only if*

$$(i) \qquad X^{[k]}\left(F\left(\mathbf{x}, u, u_1, \ldots, u_k\right)\right)\big|_{F=0} = 0; \tag{5.8}$$

$$(ii) \qquad X\omega_\alpha(\mathbf{x})\big|_{\omega_\alpha(\mathbf{x})=0} = 0; \tag{5.9}$$

$$(iii) \quad X^{[k-1]}B_\alpha\left(\mathbf{x}, u, u_1, \ldots, u_{k-1}\right)\big|_{\omega_\alpha(\mathbf{x})=0, B_\alpha=0} = 0. \tag{5.10}$$

for $\alpha = 1, 2, 3, \ldots, s$.

Definition 1 leads to the following theorem:

Theorem 1 *Let BVP (5.4)-(5.6) admit the generator of infinitesimal transformations (5.7). Let* $\mathbf{\Theta} = (X_1(\mathbf{x}), X_2(\mathbf{x}), \ldots, X_{n-1}(\mathbf{x}))$ *be* $n-1$ *group invariants of (5.7) depending only on* $\mathbf{x}$*. Let* $v(\mathbf{x}, u)$ *be a group invariant of (5.7) such that* $\partial v/\partial u \neq 0$*. Then the BVP (5.4)-(5.6) reduces to*

$$G\left(\mathbf{\Theta}, v, v_1, v_2, \ldots, v_k\right) = 0 \tag{5.11}$$

defined on some domain $\Omega_{\mathbf{X}}$ *in* $\mathbf{X}$*-space with boundary conditions*

$$C_\alpha\left(\mathbf{\Theta}, v, v_1, \ldots, v_k\right) = 0 \tag{5.12}$$

on prescribed boundary surfaces

$$\nu_\alpha\left(\mathbf{\Theta}\right) = 0, \tag{5.13}$$

for some G, C_α, ν_α, $\alpha = 1, 2, \ldots, s$.

Theorem 1 is proved in Bluman and Kumei [13].

For the problem under consideration in this thesis we consider the general boundary values:

$$x = a, \qquad y(a) = b, \qquad y'(a) = c. \tag{5.14}$$

For general k Bozkhov and Martins [16, 43] have shown that (5.1) admits the infinitesimal generator

$$X = x\frac{\partial}{\partial_x} - 2\frac{\partial}{\partial_y}. \tag{5.15}$$

A first extension is given by

$$X^{[1]} = x\frac{\partial}{\partial x} - 2\frac{\partial}{\partial y} - y'\frac{\partial}{\partial y'}. \tag{5.16}$$

Then from Definition 1 and Theorem 1 we have to solve the system of equations

$$X^{[1]}\left(x-a\right)\big|_{x=a} = 0, \qquad X^{[1]}\left(y-b\right)\big|_{x=a,y=b} = 0,$$

$$X^{[1]}\left(y'-c\right)\big|_{x=a,y=b,y'=c} = 0. \tag{5.17}$$

We can ignore the condition supplied by the dependent variable y since it does not give us any new insights. The equation $-2 = 0$ supplied by this case does not lead to any inconsistencies since the boundary conditions (5.14) are general and hence the -2 may just be incorporated into the constant b. We find that

$$x = 0, \qquad y' = 0. \tag{5.18}$$

Applying the invariance principle does not give a condition on $y(0)$. Therefore for general k the only invariant boundary condition is given by

$$y'(0) = 0. \tag{5.19}$$

Invariants corresponding to (5.16) are given by [21, 25, 16]

$$u = x^2 e^y, \qquad v = xy'. \tag{5.20}$$

These invariants reduce (5.1) to the first-order ordinary differential equation

$$\frac{dv}{du} = \frac{v(1-k) - \delta u}{u(v+2)}. \tag{5.21}$$

The boundary condition (5.19) implies that

$$v(0) = 0. \tag{5.22}$$

5.3 Dynamical systems analysis

For general k we write the first-order ordinary differential equation (5.21) as the autonomous system

$$\frac{dv}{dt} = v(1-k) - \delta u, \qquad \frac{du}{dt} = u(v+2) \tag{5.23}$$

where $u(0) = 0$ and $v(0) = 0$. The system (5.23) for $k \neq 1$ has stationary points z_1 and z_2 given by

$$z_1 = (0, 0), \qquad z_2 = \left(\frac{2(k-1)}{\delta}, -2\right). \tag{5.24}$$

We now consider a linear stability analysis to classify the stationary points. For $k = 1$ all points on the line $u = 0$ are stationary for (5.23).

The Jacobian matrix J for the system (5.23) is given by

$$J(u,v) = \begin{bmatrix} -\delta & 1-k \\ 2+v & u \end{bmatrix}. \tag{5.25}$$

Evaluating J at z_1 we find that

$$J(0,0) = \begin{bmatrix} -\delta & 1-k \\ 2 & 0 \end{bmatrix} \tag{5.26}$$

with corresponding eigenvalues

$$\lambda_{1,2} = \frac{1}{2}\left(-\delta \pm \sqrt{8+\delta^2-8k}\right). \tag{5.27}$$

The eigenvalues are real provided

$$k \leq \frac{1}{8}\left(8+\delta^2\right). \tag{5.28}$$

For

$$k = \frac{1}{8}\left(8+\delta^2\right) \tag{5.29}$$

the resulting eigenvalues are $\lambda_1 = \lambda_2 = -\delta/2$ which indicates that there is only one independent eigenvector. Therefore for $\delta < 0$ the eigenvalues are positive and the trajectories are repelled from the stationary point z_1 in the shape of a spiral. For $\delta > 0$ the eigenvalues are negative and the trajectories tend to z_1 in an asymptotically stable spiral. For

$$k < \frac{1}{8}\left(8+\delta^2\right) \tag{5.30}$$

the eigenvalues λ_1 and λ_2 are real but unequal. For $k > 1$ and $\delta < -\sqrt{8k-8}$ the stationary point z_1 is an unstable node. For $k > 1$ and $\delta > -\sqrt{8k-8}$ the stationary point z_1 is asymptotically stable with trajectories tending to z_1 in a spiral. For

$$k > \frac{1}{8}\left(8+\delta^2\right) \tag{5.31}$$

the eigenvalues λ_1 and λ_2 are imaginary with the sign of the real part depending on the sign of $-\delta/2$. For $\delta < 0$ the real part of the eigenvalues are positive and the stationary point z_1 is unstable. Trajectories move away from the stationary z_1 in the shape of a

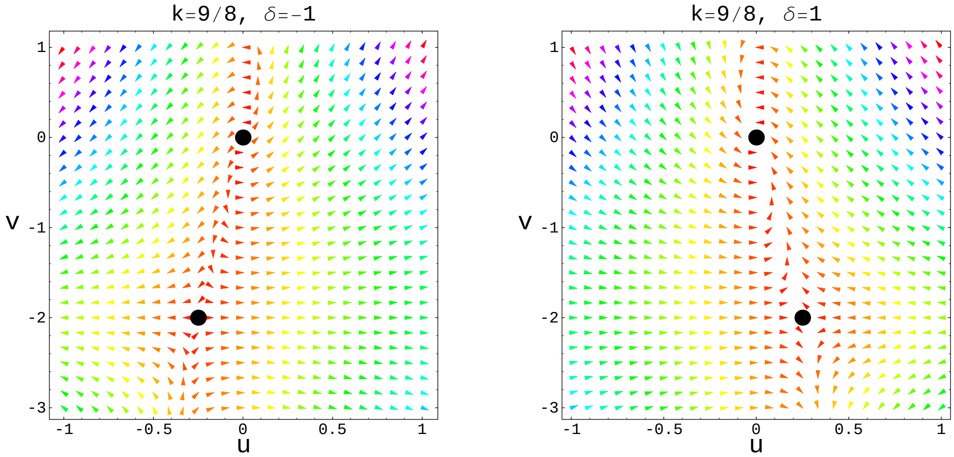

Figure 5.1: *Plot of the phase trajectories for the system (5.23) with* $k = \frac{1}{8}(8 + \delta^2)$ *for the cases* $\delta = -1$ *and* $\delta = 1$.

spiral. For $\delta > 0$ the real part of the eigenvalue is negative and the trajectories tend to the stationary point z_1 in an asymptotically stable spiral pattern.

As an example of these trajectories we consider the case where k is given by (5.29) and $\delta = \pm 1$. For $\delta = -1$ we observe in Figure 5.1 that the trajectories are moving away from the stationary point z_1 in a spiral pattern while for $\delta = 1$ the trajectories approach z_1 in a spiral pattern. The stationary point z_2 is an unstable stationary point for both the cases indicated in Figure 5.1, since the trajectories are deflected from the stationary point.

Evaluating J at z_2 we find that

$$J\left(\frac{2(k-1)}{\delta}, -2\right) = \begin{bmatrix} -\delta & 1-k \\ 0 & \dfrac{2(k-1)}{\delta} \end{bmatrix} \tag{5.32}$$

with corresponding eigenvalues

$$\lambda_3 = -\delta, \qquad \lambda_4 = \frac{2(k-1)}{\delta}. \tag{5.33}$$

The eigenvalues λ_3 and λ_4 are always real. For $k = (1/2)(2 - \delta^2)$ where $\delta \neq 0$ the eigenvalues, λ_3 and λ_4, are equal to $-\delta$. The stationary point z_2 then becomes

$$z_3 = (-\delta, -2). \tag{5.34}$$

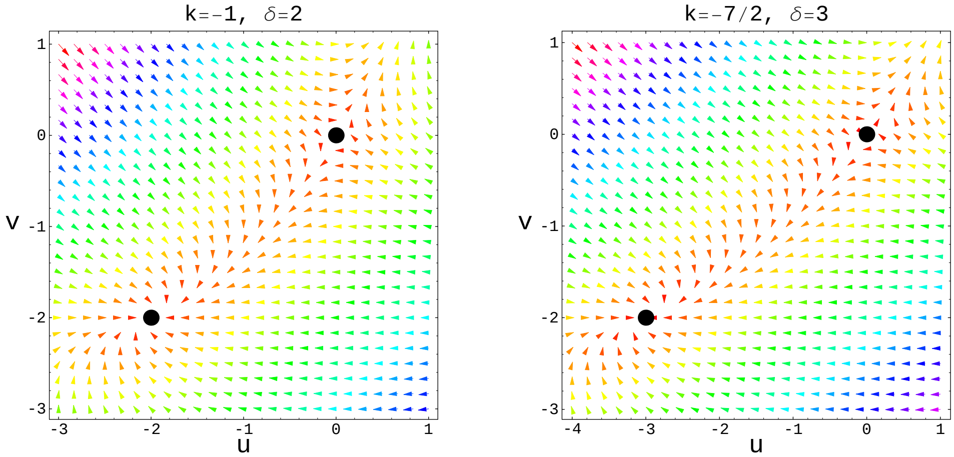

Figure 5.2: *Plot of the phase trajectories for the system (5.23) for $k = -1$ with $\delta = 2$ and $k = -7/2$ with $\delta = 3$ indicating that the trajectories are deflected from z_1 and tend to z_2 in a stable spiral.*

For $\delta > 0$ the eigenvalue is negative but there is only one independent eigenvector hence trajectories tend to z_3 in an asymptotically stable spiral and $(0, 0)$ is an asymptotically stable improper node. For $\delta < 0$ the eigenvalue is positive with only one independent eigenvector hence the point z_3 is an unstable node and z_1 is also unstable. In Figure 5.2 we plot phase diagrams indicating that z_1 is an unstable node and z_2 is stable.

The stability analysis performed here is critical in terms of a numerical solution to (5.1). We have shown using a symmetry approach that for general k the boundary condition $y' = 0$ on the line $x = 0$ is an invariant boundary condition. From the phase plane analysis above we can conclude that for $\delta > 0$ and $k \leq 1$ the boundary condition $y' = 0$ is unstable on the line $x = 0$. While for $\delta > 0$ and $k > 1$ the boundary condition $y' = 0$ is stable on the line $x = 0$. We plot phase diagrams of the system (5.23) for $\delta = 1$ and $k = 0, 1, 2$ in Figure 5.3, which supports our conclusion. In Figure 5.3 for $k = 0$ and $k = 1$ we observe that the point z_1 is unstable and the trajectories z_1 are deflected. For $k = 2$ the trajectories tend to the stable stationary point z_1 in a spiral. This observation of the dependence of the stability of the invariant boundary condition on the shape factor is critical in the numerical solution of the boundary value problem (5.1) solved subject to (5.2).

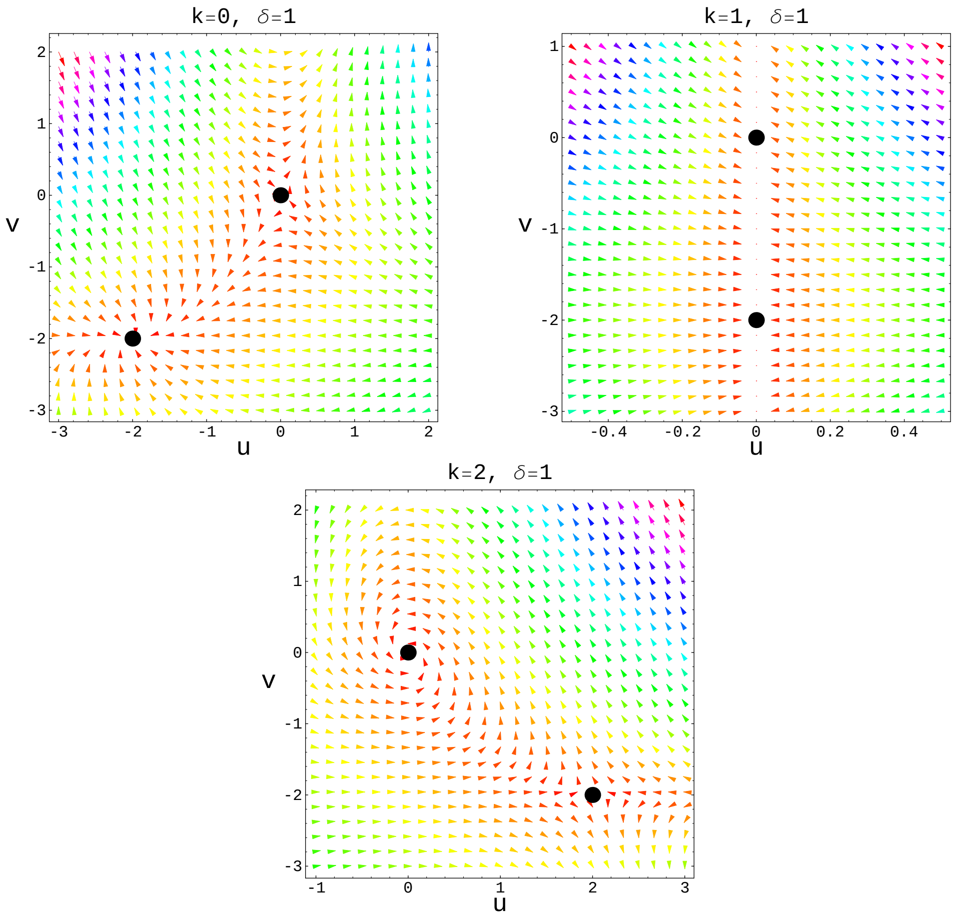

Figure 5.3: *Plot of the phase trajectories for the system (5.23) for* $\delta = 1$ *and* $k = 0, 1, 2$.

5.3.1 Invariant boundary conditions for the case $k = 1$

The case for $k = 1$ has been solved in Chapter 4 [35] where the model described the thermal explosion within a cylindrical vessel. However we wish to use the invariant boundary condition (5.19) discovered in Section 5.2. To make analytical progress in solving (5.21) using this invariant boundary condition we consider the case $k = 1$ for equation (5.1) which admits the additional infinitesimal generator

$$Y = x(\ln x - 1)\frac{\partial}{\partial x} - 2\ln x\frac{\partial}{\partial y}. \tag{5.35}$$

Using this Lie point symmetry (5.35) the first-order ordinary differential equation (5.21) reduces to the separable equation

$$(v + 2)dv = -\delta du. \tag{5.36}$$

Integrating (5.36) and imposing (5.22) we find that

$$(v + 2)^2 = 4 - 2\delta u. \tag{5.37}$$

Substituting (5.20) into (5.37) we obtain the first-order ordinary differential equation

$$y'^2 + \frac{4}{x}y' + 2\delta e^y = 0. \tag{5.38}$$

Solving (5.38) we obtain the solutions

$$y = \ln\left[\frac{16e^{c_1}}{(2\delta + e^{c_1}x^2)^2}\right], \qquad y = \ln\left[\frac{16e^{c_2}}{(1 + 2\delta e^{c_2}x^2)^2}\right] \tag{5.39}$$

where c_1 and c_2 are constants of integration, [25].

Equation (5.21) for the case $k = 1$ admits the additional infinitesimal generator (5.35). A first-order extension of (5.35) is given by

$$Y^{[1]} = x(\ln x - 1)\frac{\partial}{\partial x} - 2\ln x\frac{\partial}{\partial y} - \left(\frac{2}{x} + y'\ln x\right)\frac{\partial}{\partial y'}. \tag{5.40}$$

We consider the following

$$Y^{[1]}(x - a)\big|_{x=a} = 0, \qquad Y^{[1]}(y - b)\big|_{x=a,y=b} = 0,$$

$$Y^{[1]}\left(y'-c\right)\Big|_{x=a,y=b,y'=c}=0 \tag{5.41}$$

and upon solving (5.41) we find that

$$x=e, \qquad y'(e)=-\frac{2}{e}. \tag{5.42}$$

Once again we do not get a condition on $y(e)$. Therefore, in terms of symmetries, the natural choice of boundary conditions to be used for solving (5.1) for the case $k=1$ are

$$y'(0)=0, \qquad y'(e)=-\frac{2}{e}. \tag{5.43}$$

We note that the second equation yields $-2logx=0$ which gives $x=1$. However we already have a condition that needs to be satisfied at this value of x. We have however found a new boundary condition which we choose to consider.

In terms of the invariants (5.20), the symmetry generator (5.40) becomes

$$\tilde{Y}=2u\frac{\partial}{\partial u}+(v+2)\frac{\partial}{\partial v}. \tag{5.44}$$

From (5.44) we obtain the new invariant

$$U=\frac{(v+2)^2}{u}. \tag{5.45}$$

Writing (5.21) for $k=1$ in terms of the new invariant we obtain the first-order ordinary differential equation

$$u\frac{dU}{du}+U+2\delta=0. \tag{5.46}$$

The first-order ordinary differential equation (5.46) is easily integrated to yield

$$U=\frac{c_3}{u}-2\delta \tag{5.47}$$

where c_3 is a constant. Substituting (5.45) into (5.47) we obtain the solution

$$(v+2)^2=c_3-2\delta u. \tag{5.48}$$

The solution (5.48) reduces to (5.37) on imposing (5.22). Imposing the boundary condition (5.43) on (5.39) we obtain the solution

$$y=2+\ln\left[\frac{8}{\delta(e^2+x^2)^2}\right]. \tag{5.49}$$

The boundary conditions (5.43) are relevant only for the case $k = 1$ and are not considered further.

It has been shown by Bozkhov and Martins [16] that X (5.15) is a Noether symmetry of (5.1). This implies that we can use Noether's theorem [53] to obtain a first-integral of (5.1) that admits X (5.15). This fact is used by Dresner [25] to obtain a first-integral for the first-order reduction of the case $k = 1$ and then to obtain an analytical solution.

5.4 Numerical solution

The model equation (5.1) is singular on the line $x = 0$. If we consider equation (5.1) close to x for a finite solution we may substitute in

$$y = a_0 + a_1 x + a_2 x^2 + \cdots \tag{5.50}$$

which gives us the following

$$\begin{gathered} a_1 = 0 \\ (2a_2(1+k) + \delta e^{a_0})x^0 + (\cdots)x = 0. \end{gathered} \tag{5.51}$$

Equivalently we are able to approximate (5.1) at $x = 0$ by

$$y''(1+k) + \delta e^y = 0 \tag{5.52}$$

to first-order for x close to zero. Since we may write $d(y')/dx = y'(dy'/dy)$ equation (5.52) can be rewritten as

$$y' \frac{dy'}{dy}(1+k) + \delta e^y = 0. \tag{5.53}$$

Therefore we find that

$$y'^2 = \alpha - \frac{2\delta}{(1+k)} e^y \tag{5.54}$$

where α is constant. It is important to note that we consider the finite solution only and not the singular case. The approximation (5.52) at $x = 0$ imposes a consistency criteria for initial values at $x = 0$ given by (5.54), i.e. only initial values of y and y' at $x = 0$ that satisfy (5.54) will iterate. Initial values that do not satisfy (5.54) will cause

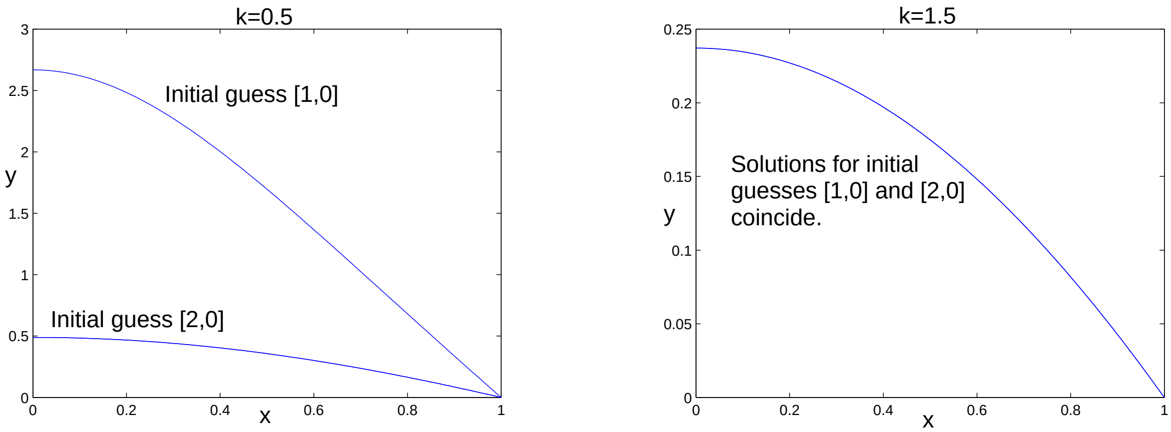

Figure 5.4: *Numerical solution of (5.1) solved subject to (5.2) using* `bvp4c` *in MATLAB for two different initial guesses* $[1, 0]$ *and* $[2, 0]$ *for* $\delta = 1$*,* $k = 0.5$ *and* $k = 1.5$*.*

the numerical calculation to terminate. By separating the equation obtained in (5.51) by powers of x we find that $a_0 = \delta e^{a_0}/(1 + k)$. Since the boundary condition $y'(0) = 0$ must hold we find that the first-order ordinary differential equation (5.54) is valid for $\alpha = a_2$.

We consider two approaches in solving the boundary value problem (5.1) solved subject to (5.2) using `bvp4c` in MATLAB. Firstly we supply initial guesses to the initial height and gradient. These initial guesses are given by the vectors $[1, 0]$ and $[2, 0]$. In Figure 5.4 we plot the numerical solutions for $k = 1$ and $k = 2$ subject to the initial guesses indicated. We note that for the case $k = 0.5$ the solution tends to two different values of the initial height. For $k = 1.5$ even though we have used two different guesses we obtain the same initial height. This immediately demonstrates the difficulty that the instability of $y' = 0$ at $x = 0$ may cause.

Instead of choosing initial points we choose a suitable initial function as a guess, [61]. We choose the function

$$y = c\left(1 - x^2\right) \tag{5.55}$$

that satisfies the boundary condition $y' = 0$ on $x = 0$ as our initial guess. The constant c is a guess to the initial height. Once again we note that for $k = 0.5$ we get two different values for the initial height depending on the value of the constant c while for

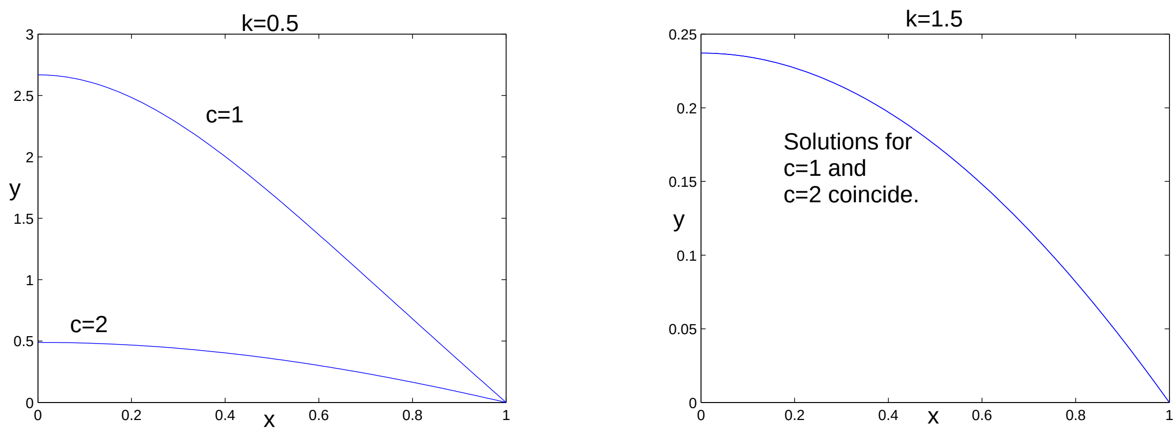

Figure 5.5: *Numerical solution of (5.1) solved subject to (5.2) using (5.55) as an initial guess for* `bvp4c` *in MATLAB where $\delta = 1$, $k = 0.5$ and $k = 1.5$.*

$k = 1.5$ we only get one. Even with making a better estimate to the solution we note how the instability of $y' = 0$ and $x = 0$ can manifest.

The instability of $y' = 0$ on $x = 0$ does not manifest when solving the initial value problem (5.1) subject to (5.3). We demonstrate this by considering a numerical solution of the initial value problem $x = 0$, $y =$ constant and $y' = 0$ and plotting the corresponding phase diagram. To view the full phase space we write (5.1) as the system of three first-order ordinary differential equations

$$\frac{dx}{dt} = 1, \quad \frac{dy}{dt} = z(t), \quad \frac{dz}{dt} = \begin{cases} -\frac{\delta e^{y(t)}}{k+1}, & x = 0, \\ -\frac{k}{x(t)} z(t) - \delta e^{y(t)}, & x \neq 0. \end{cases} \tag{5.56}$$

The system (5.56) is solved subject to the initial conditions

$$x(0) = 0, \qquad y(0) = \text{constant}, \qquad z(0) = 0. \tag{5.57}$$

From Figure 5.6 we observe that as $y \to -\infty$ then $y' \to 0$ with no instability at $x = 0$.

5.5 Finite differences

In an attempt to overcome the instability of $y' = 0$ at $x = 0$ we consider a central difference approximation to the derivatives in (5.1). The averaging of the central

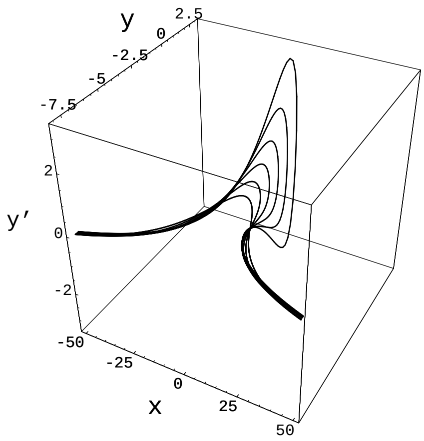

Figure 5.6: *Plot of the numerical solution of (5.56) solved subject to the initial conditions given by (5.57) for* $y(0) = -2, -1, 0, 1, 2, 3$.

difference approximation seems to prevent the discrepancy in initial height values for $k \leq 1$ irrespective of the choice of constant c in the initial guess (5.55). The proposed scheme does not work for the case $k = 0$. The scheme has to be rewritten for the second-order ordinary differential equation as follows

$$y'' + \delta e^y = 0. \tag{5.58}$$

For our numerical scheme we consider a partition on the domain $[a, b]$ by segmenting the domain into $n + 1$ equidistant steps

$$a = x_0 < x_1 < x_2 < \ldots < x_{n-1} < x_n = b \tag{5.59}$$

where $y_i = y(x_i)$ and where we approximate derivatives at x_i by the central differences

$$y' \approx \frac{y_{i+1} - y_{i-1}}{2h}, \qquad y'' \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}. \tag{5.60}$$

We approximate (5.1) at $x = 0$ by (5.52). We then solve the coupled system (5.52) and (5.1) on the domain $[a, b] = [0, 1]$ for boundary conditions (5.2). The boundary conditions (5.2) imply that

$$y_{-1} = y_1, \qquad y_n = 0. \tag{5.61}$$

The resulting nonlinear system of equations we have to solve is given by

$$\begin{bmatrix} -2 & 2 & 0 & 0 & \dots & 0 & 0 & 0 \\ \alpha_1 & -2 & \beta_1 & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \alpha_2 & -2 & \beta_2 & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \alpha_{n-1} & -2 & \beta_{n-1} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{bmatrix} = -\delta h^2 \begin{bmatrix} \frac{1}{(1+k)} e^{y_0} \\ e^{y_1} \\ e^{y_2} \\ \vdots \\ e^{y_{n-1}} \\ 0 \end{bmatrix} \tag{5.62}$$

where

$$\alpha_i = \left(1 - \frac{kh}{2x_i}\right), \qquad \beta_i = \left(1 + \frac{kh}{2x_i}\right). \tag{5.63}$$

The system (5.62) is reduced to a linear system by writing it as

$$\begin{bmatrix} -2 & 2 & 0 & 0 & \dots & 0 & 0 & 0 \\ \alpha_1 & -2 & \beta_1 & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \alpha_2 & -2 & \beta_2 & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \alpha_{n-1} & -2 & \beta_{n-1} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y_0^{(i+1)} \\ y_1^{(i+1)} \\ y_2^{(i+1)} \\ \vdots \\ \vdots \\ y_{n-1}^{(i+1)} \\ y_n^{(i+1)} \end{bmatrix} = -\delta h^2 \begin{bmatrix} \frac{1}{(1+k)} e^{y_0^{(i)}} \\ e^{y_1^{(i)}} \\ e^{y_2^{(i)}} \\ \vdots \\ \vdots \\ e^{y_{n-1}^{(i)}} \\ 0 \end{bmatrix} \tag{5.64}$$

where we assume an initial **y** vector with components given by

$$y_i^{(0)} = c\left(1 - x_i^2\right). \tag{5.65}$$

From Figure 5.7 we note that the solutions for $k = 0.5$ and $k = 1$ follow the trend of a decreasing initial height as the value of k increases. However, for the initial values in Figures 5.5 and 5.6 there are two values of the initial height obtained for values of $k \leq 1$. The numerical solution for $k = 1$ does in fact match the analytical solution obtained by Frank-Kamenetskii [29] and Chambré [21]. Other approaches for solving boundary value problems are presented in Ascher et al. [8] and may also prove useful in finding approaches that can circumvent the instability of $y' = 0$ on $x = 0$ for $k \leq 1$.

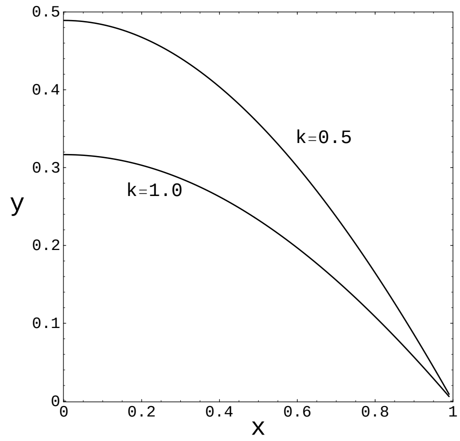

Figure 5.7: *Numerical solution of (5.1) solved subject to (5.2) for* $n = 100$*,* $\delta = 1$*,* $k = 0.5$ *and* $k = 1$*.*

5.6 Analytical attainment of an initial guess

We note that (5.1) has two parameters, δ and k. To make analytical progress in determining a suitable initial guess for the numerical scheme considered in the Section above, we assume that

$$\delta = O(k). \tag{5.66}$$

The model equation (5.1) can then be written as

$$y'' + \frac{k}{x}y' + ke^y = 0. \tag{5.67}$$

We investigate an approximate solution admitted by (5.67) of the form

$$y = G_0(x) + kG_1(x) + \cdots, \qquad k \ll 1. \tag{5.68}$$

The exponential term can be written as

$$e^{G_0(x)+kG_1(x)+k^2G_2(x)\cdots} = e^{G_0(x)}e^{kG_1(x)}e^{k^2G_2(x)}\cdots \qquad k \ll 1. \tag{5.69}$$

Since the parameter k is suitably small we have that $|kG_1(x)| \ll 1$. This enables us to approximate the exponential term as follows

$$e^y \approx e^{G_0(x)}(1 + kG_1(x)), \qquad k \ll 1. \tag{5.70}$$

Substituting (5.68) into (5.67) and separating by coefficients of k we obtain the system of equations

$$G_0'' = 0, \qquad G_1'' + \frac{G_0'}{x} + e^{G_0} = 0. \tag{5.71}$$

Solving the system (5.71) and imposing the boundary conditions

$$G_0'(0) = G_1'(0) = 0, \qquad G_0(1) = G_1(1) = 0 \tag{5.72}$$

obtained from (5.2) we find that

$$y = -\frac{1}{2}k(x^2 - 1), \qquad k \ll 1. \tag{5.73}$$

Dividing (5.67) by k we obtain

$$\frac{1}{k}y'' + \frac{1}{x}y' + e^y = 0. \tag{5.74}$$

For large k we determine an approximate solution of the form

$$y = F_0(x) + \frac{1}{k}F_1(x) + \dots, \qquad \frac{1}{k} \ll 1. \tag{5.75}$$

Substituting (5.75) into (5.74) and separating by coefficients of $1/k$ we obtain the system

$$\frac{F_0'}{x} + e^{F_0} = 0, \qquad \frac{F_1'}{x} + F_1 e^{F_0} + F_0'' = 0. \tag{5.76}$$

Solving the system (5.76) subject to

$$F_0'(0) = F_1'(0) = 0, \qquad F_0(1) = F_1(1) = 0 \tag{5.77}$$

we find that

$$y = \log\left[\frac{2}{1+x^2}\right] + \frac{1}{k}\left(\frac{1 - x^2 + 2\log\left[\frac{1+x^2}{2}\right]}{1+x^2}\right) \qquad \frac{1}{k} \ll 1. \tag{5.78}$$

Using (5.73) for $k \ll 1$ and (5.78) for $\frac{1}{k} \ll 1$ as initial guesses in a package like `bvp4c` in MATLAB [61] is another way of overcoming the instability of the boundary condition $y'(0) = 0$ for $k \le 1$.

5.7 Concluding Remarks

In this Chapter we have shown how the Lie group method provides a useful tool for discovering invariant boundary conditions. Using a dynamical systems analysis we were able to investigate the stability of these invariant boundary conditions. For the Lane-Emden equation of the second-kind (5.1) we note that the stability of the boundary condition $y' = 0$ on $x = 0$ changes from stable for shape factor $k > 1$ to unstable for $k \leq 1$. We have verified this by using the program `bvp4c` in MATLAB to solve (5.1) subject to (5.2) for different values of k. We have also shown that this instability does not manifest when solving an initial value problem. We were able to overcome the instability by using a central difference approximation to the derivatives in our model equation. The occurrence of this instability is not obvious since the method of central differences which is used to overcome the instability is the most commonly used method to solve boundary value problems.

One possible problem with the initial guess (5.55) may be that it is a polynomial while analytical solutions obtained by Frank-Kamenetskii [29] and Chambré [21] are logarithmic. Using a logarithmic initial guess may prove useful for the numerical algorithm `bvp4c` in MATLAB. One would then have to contend with derivatives not existing at particular points. We do note however that without knowing the form of an analytical solution a priori a polynomial as a guess is still a better approach.

In Section 5.6 we have given another efficient way of calculating initial guesses to the boundary value problem (5.1) solved subject to (5.2) that can be used in a package like `bvp4c` in MATLAB [61]. Two initial guesses are given for different ranges of k. This initial guess (5.73) is similar to the one obtained previously (5.65) and also overcomes the instability of the boundary condition $y'(0) = 0$ for $k \leq 1$. The initial guess (5.78) is an appropriate initial guess for $k > 1$.

Chapter 6

First integrals and bifurcations of a Lane-Emden equation of the second-kind

Some of the work in this Chapter has appeared in:

Harley, C. and Momoniat, E., *First integrals and bifurcations of a Lane-Emden equation of the second-kind*, Journal of Mathematical Analysis and Applications, 344, (2008), 757–764.

As done in previous Chapters we investigate first integrals admitted by a Lane-Emden equation modelling a thermal explosion in a rectangular slab and cylindrical vessel. A perturbation is introduced into the equation via the small parameter ϵ. By imposing the boundary conditions on the first integrals we obtain a nonlinear relationship between the temperature at the center of the vessel and the temperature gradient at the wall of the vessel. For a rectangular slab we note the presence multiple values for the temperature at the center of the vessel when the temperature gradient at the wall is fixed. For a cylindrical vessel we find multiple values for the temperature gradient at the walls of the vessel when the temperature at the center of the vessel is fixed. In both of these relationships we notice the presence of the perturbation parameter. In this Chapter any reference made to the occurrence of a bifurcation is a comment on the presence of multiple values. In particular what is meant by bifurcation in this Chapter is the occurrence of multiple values at a specific boundary.

6.1 Introduction

In Section 4.4 we found a relationship between the temperature gradient at the wall and the temperature at the center of the cylindrical vessel. However we had assumed the parameter ϵ in equation (6.1) to be zero. In this Chapter we investigate such relationships between parameters by considering the following perturbed Lane-Emden equation of the second-kind

$$y'' + \frac{k}{x}y' + \delta \exp\left(\frac{y}{1+\epsilon y}\right) = 0, \qquad \epsilon \ll 1 \tag{6.1}$$

where $' = d/dx$ with δ a constant known as the Frank-Kamenetskii [29] parameter. In this way relationships between parameters will also include terms of ϵ. The boundary conditions for the thermal explosion problem in a rectangular geometry are given by

$$y(\pm 1) = 0 \tag{6.2}$$

and for a cylindrical geometry they are given by

$$y'(0) = 0, \qquad y(1) = 0. \tag{6.3}$$

We consider approximate first integrals admitted by the perturbed Lane-Emden equation (6.1) which models a thermal explosion in a rectangular slab and cylindrical vessel. By imposing the boundary conditions (6.3) on the first integrals we obtain a nonlinear relationship between the temperature at the center of the vessel and the temperature gradient at the wall of the vessel. By imposing the boundary conditions (6.2) and (6.3) we note the presence of bifurcations in a rectangular and cylindrical vessel.

The constant ϵ has thus introduced the existence of bifurcations at the boundaries of the vessels.

6.2 Approximate first integrals

The theoretical work introduced in this Section is discussed in more detail in Chapter 2. We will use a direct approach for constructing first integrals. To simplify calculations for this procedure we first approximate the power of the exponential function in equation (6.1). We use the fact that $\epsilon \ll 1$ to simplify (6.1). Using the approximation

$$\frac{y}{1+\epsilon y} = y - \epsilon y^2 + \epsilon^2 y^3 - \epsilon^3 y^4 + \cdots \tag{6.4}$$

we simplify (6.1) to

$$y'' + \frac{k}{x}y' + \delta e^{\left(y-\epsilon y^2\right)} = 0 \tag{6.5}$$

valid to first-order in ϵ. By expanding the exponential function we can simplify (6.5) further to

$$y'' + \frac{k}{x}y' + \delta e^{y}\left(1-\epsilon y^2\right) = 0. \tag{6.6}$$

It is easily seen that the original exponential term $e^{\frac{y}{1+\epsilon y}}$ is monotonic and the approximation thereof, given by $e^{y}\left(1-\epsilon y^2\right)$, is not. However in considering the domain upon which these functions coincide it is clear that the value of ϵ is important. As the value of ϵ diminishes so does the domain for y upon which the functions correspond to each other increase. Since it is assumed that $\epsilon \ll 1$ it seems conceivable that in this context the approximation applied to obtain equation (6.6) is reasonable. It is noted that for $\epsilon = 0.05$ the domain for y is greater than $[0, 1]$ which is appropriate considering the boundary conditions that our equation adheres to.

6.2.1 Infinite rectangular slab (k = *0*)

For the case $k = 0$ equation (6.6) reduces to the autonomous equation

$$y'' + \delta e^{y}\left(1-\epsilon y^2\right) = 0. \tag{6.7}$$

In this Chapter we investigate approximate first integrals of the form

$$I = I_0 + \epsilon I_1. \tag{6.8}$$

In Chapter 4 [37] we showed that the unperturbed equation from (6.7) admits the first integral

$$I_0 = y'^2 + 2\delta e^y. \tag{6.9}$$

To determine I_1 we take the total derivative of (6.8), i.e.

$$D_x \left(I_0 + \epsilon I_1\right)\big|_{(6.6)} = O\left(\epsilon^2\right) \tag{6.10}$$

where the total differentiation operator D_x is defined by (2.48). Since the equation (6.7) is autonomous we can write equation (6.10) as

$$D_x I = y'(I_0)_y + y'\epsilon(I_1)_y - \delta e^y(1-\epsilon y^2)(I_0)_{y'} - \epsilon\delta e^y(1-\epsilon y^2)(I_1)_{y'} \tag{6.11}$$

where subscripts denote differentiation. Substituting in I_0 as defined by (6.9) and separating by coefficients of powers of ϵ we solve the resulting system of equations to obtain

$$I_1 = -2\delta e^y\left(y^2 - 2y + 2\right). \tag{6.12}$$

Therefore from (6.8) we have that

$$I = y'^2 + 2\delta e^y - 2\epsilon\delta e^y\left(y^2 - 2y + 2\right). \tag{6.13}$$

Typically, we would solve

$$I = C = \text{constant} \tag{6.14}$$

to obtain a solution admitted by (6.6). Instead of doing this we impose the boundary conditions (6.2) on (6.14) where I is defined by equation (6.13) to obtain

$$y'^2(-1) = y'^2(1). \tag{6.15}$$

Equation (6.15) confirms the symmetry of the temperature gradient at the vessel walls for the rectangular geometry. We can thus impose boundary conditions (6.3) on (6.14). We find that

$$y'^2(1) = \delta\left[-2 + 4\epsilon + e^{y(0)}\left(2 - 2\epsilon\left(2 - y(0) + y(0)^2\right)\right)\right]. \tag{6.16}$$

Equation (6.16) gives a nonlinear relationship between the temperature gradient at the wall and the temperature at the centre of the rectangular vessel. In Figure 6.1 we plot (6.16) for $\epsilon = 0$. From Figure 6.1 we observe that for a fixed δ we can control the temperature at the centre of the vessel by controlling the temperature gradient at the vessel wall. Increasing values of δ decreases the maximum possible temperature at the centre of the vessel. This result was obtained in Chapter 4 [37].

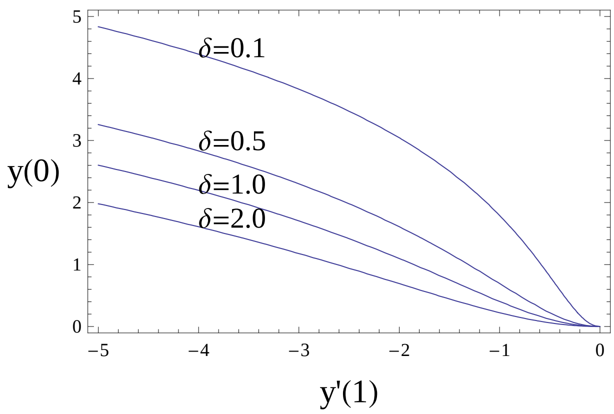

Figure 6.1: *Plot of the temperature at the center of the rectangular slab as a function of the temperature gradient at the wall for* $\epsilon = 0$.

In Figure 6.2 we plot (6.16) for $\epsilon = 0.05$ and $\epsilon = 0.1$. From Figure 6.2 we observe that nonzero values of ϵ introduce multiple values of $y(0)$. The bifurcation in Figure 6.2 gives multiple values for the temperature at the center of the vessel when the temperature gradient at the walls of the vessel is fixed.

6.2.2 Infinite circular cylinder (k = *1*)

For $k = 1$ (6.6) reduces to

$$y'' + \frac{1}{x}y' + \delta e^y \left(1 - \epsilon y^2\right) = 0. \tag{6.17}$$

Using the results from [16, 53, 37] we find that the unperturbed equation from (6.17) admits the first integral

$$I_0 = \frac{1}{2}x^2 y'^2 + 2xy' + \delta x^2 e^y. \tag{6.18}$$

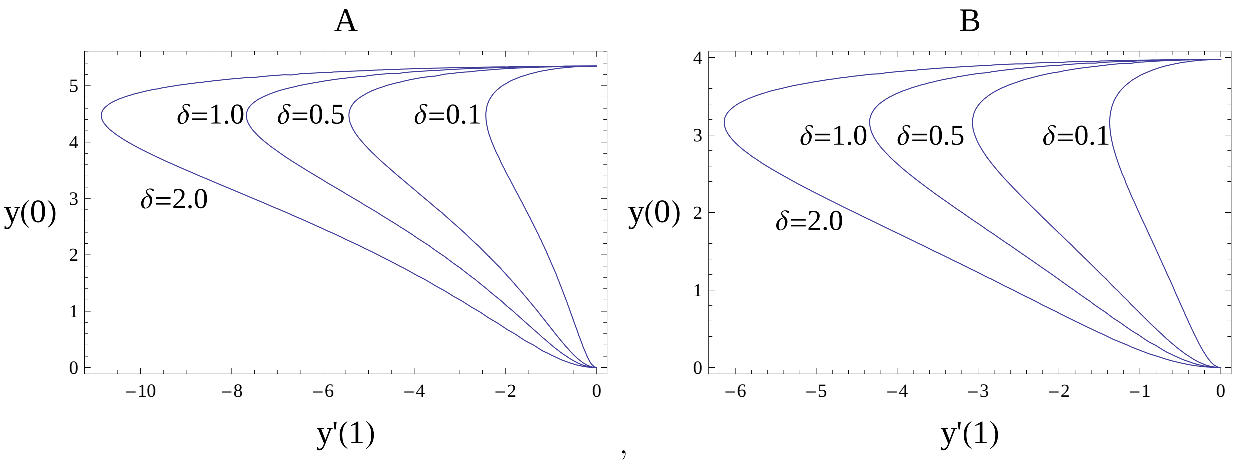

Figure 6.2: *Plot of the temperature at the center of the rectangular slab as a function of the temperature gradient at the wall for* $\epsilon = 0.05$ *(A) and* $\epsilon = 0.1$ *(B).*

We calculate I_1 using the same approach as described for the case $k = 0$. We consider the equation

$$D_x I = (I_0)_x + (I_1)_x + y'(I_0)_y + y'\epsilon(I_1)_y$$
$$-(\frac{k}{x}y' + \delta e^y(1 - \epsilon y^2))(I_0)_{y'} - \epsilon(\frac{k}{x}y'\delta e^y(1 - \epsilon y^2))(I_1)_{y'} \quad (6.19)$$

where subscripts denote differentiation. Substituting in I_0 as defined by (6.18) and separating by coefficients of powers of ϵ we obtain

$$I_1 = 16y + x\left(4y'\left(y - 3\right) - \delta x e^y\left(2 + y(y - 2)\right)\right) - 4x\left(2\delta x e^y + y'\left(4 + xy'\right)\right)\log x. \quad (6.20)$$

Once again we substitute (6.18) and (6.20) into (6.8). We substitute the resulting approximate first integral into (6.14) and impose the boundary conditions (6.3) to obtain

$$\frac{1}{2}y'^2(1) + 2y'(1) + \delta - 16\epsilon y(0) - \epsilon\left(12y'(1) + 2\delta\right) = 0. \quad (6.21)$$

We plot (6.21) in Figure 6.3 for $\epsilon = 0$. We note that instead of getting a relationship comparing the temperature at the center of the cylindrical vessel with the temperature gradient at the wall we obtain a quadratic equation showing the dependence of the temperature gradient on the critical value δ. From Figure 6.3 we note that the maximum value of δ is obtained when $y'(1) = -2$.

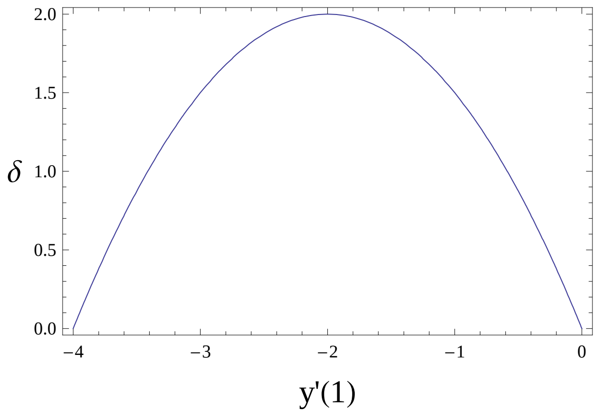

Figure 6.3: *Plot of the critical value δ as a function of the temperature gradient at the wall for $\epsilon = 0$.*

In Figure 6.4 we plot (6.21) for $\epsilon = 0.01$ and $\epsilon = 0.1$. Once again we see a bifurcation indicating multiple values for the temperature at the center of the vessel when the temperature gradient at the wall is fixed. The effects of the bifurcation for the case $k = 1$ does not manifest itself because $y'(1) < 0$ for physically meaningful solutions. These solutions lie on the bottom half of the bifurcating curves indicated in Figure 6.4.

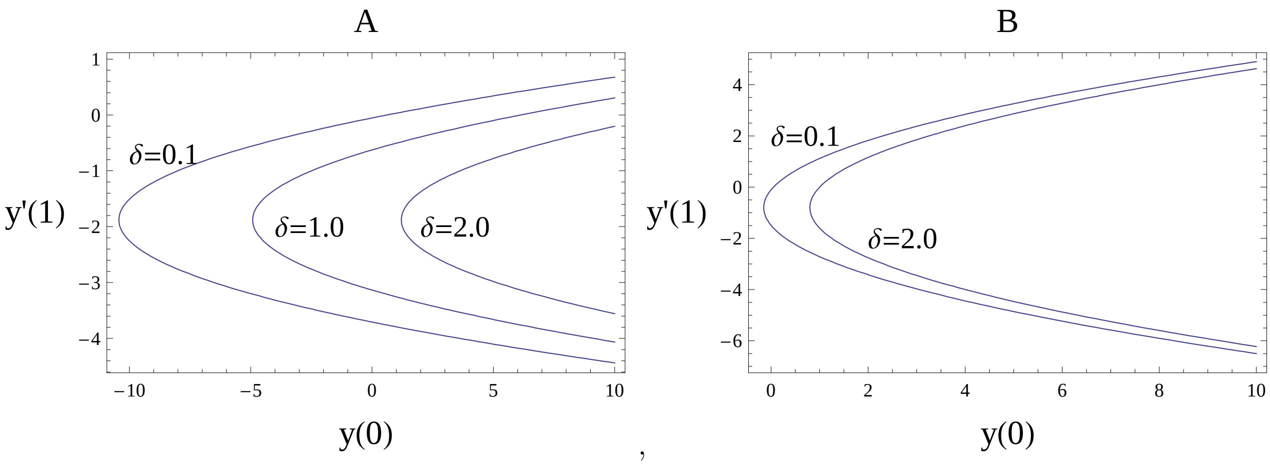

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Figure 6.4: *Plot of the temperature gradient at the wall as a function of the temperature at the center of the cylindrical vessel for $\epsilon = 0.01$ (A) and $\epsilon = 0.1$ (B).*

6.3 Concluding Remarks

In order to investigate the multiplicity of the boundary conditions of equation (6.1) we have investigated approximate first integrals admitted by the perturbed Lane-Emden equation (6.1). Equation (6.1) models a thermal explosion in a vessel with thermally conducting walls. The temperature at the center is positive because the chemical reaction is producing heat, i.e.

$$y(0) > 0. \tag{6.22}$$

The temperature at the centre of the vessel is always higher than the temperature at the walls. This implies that the temperature gradient at the walls is always negative, i.e.

$$y'(1) < 0. \tag{6.23}$$

For the case $k = 0$ and $\epsilon = 0$ no multiple values are observed. For $\epsilon \neq 0$ we observe the presence of a bifurcation. From Figure 6.2 we see that for a fixed temperature gradient at the rectangular vessel walls we get two possible values for the temperature at the center of the rectangular vessel. This bifurcation manifest itself when we consider a numerical solution of (6.1) for $k = 0$. In Figure 6.5 we plot the results obtained from a numerical solution of (6.1) obtained using `bvp4c` in MATLAB [61].

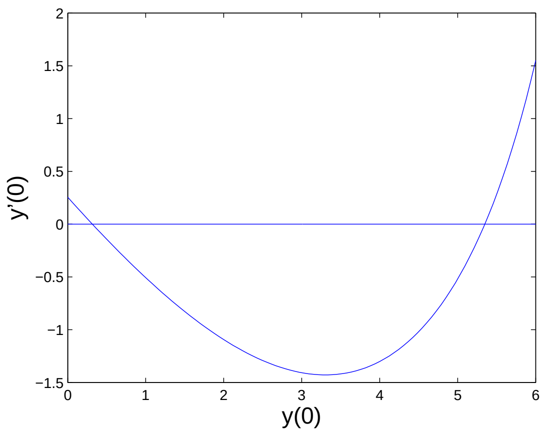

Figure 6.5: *Plot of results obtained from a numerical solution of (6.1) for $k = 0$ obtained using* `bvp4c` *in MATLAB by fixing $y(1) = 0$ for $\epsilon = 0.1$ and $\delta = 0.5$.*

The results indicated in Figure 6.5 were obtained by fixing the boundary condition $y(1) = 0$ and varying the boundary condition at $y(0)$. As $y(0)$ is varied we calculate values of $y'(0)$. We plot $y'(0)$ against $y(0)$ in Figure 6.5. From Figure 6.5 we note that there are two values of $y(0)$ that satisfy the physical boundary condition $y'(0) = 0$.

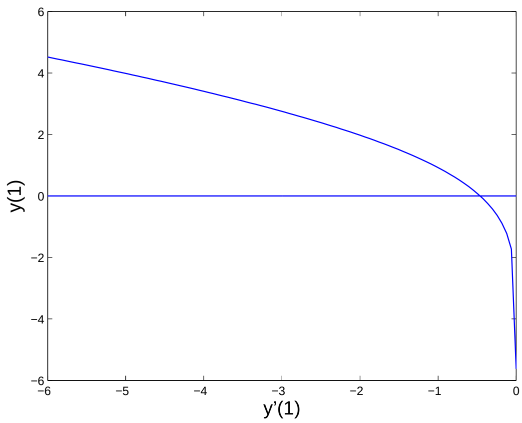

Figure 6.6: *Plot of results obtained from a numerical solution of (6.1) for $k = 0$ obtained using* `bvp4c` *in MATLAB by fixing $y'(0) = 0$ for $\epsilon = 0.1$ and $\delta = 0.5$.*

The results indicated in Figure 6.6 were obtained by fixing $y'(0) = 0$ and varying $y'(1)$. Values of $y(1)$ are calculated and we plot $y'(1)$ against $y(1)$ in Figure 6.6. Here we observe that there is only one value of $y'(1)$ that corresponds to $y(1) = 0$.

The results obtained in Figures 6.5 and 6.6 reflect the implications of the bifurcation in Figure 6.2. Multiple values of $y(0)$ exist for a fixed value of $y'(1)$ for small ϵ. The case $k = 1$ exhibits similar results for small values of ϵ. Multiple values of $y'(1)$ exist for fixed values of $y(0)$. We note from Figure 6.4 that as the value of ϵ increases the conditions (6.22) and (6.23) limit the appearance of multiple values of $y'(1)$.

Chapter 7

Implicit series solution for a boundary value problem modelling a thermal explosion

The work done in this Chapter has been submitted for publication:

Harley, C. and Momoniat, E., *Implicit series solution for a boundary value problem modelling a thermal explosion*, Computers and Mathematics with Applications, (2008).

In our final Chapter we follow up on the work done in Chapter 3 [52]. We consider the Lane-Emden equation of the second-kind as a boundary value problem. In Chapter 3 [52] we considered this equation for a shape factor of two, indicating a spherical vessel. In this Chapter we do not specify the value of the shape factor, in other words we do not specify the shape of the geometry. Through the use of a coordinate transformation introduced by Chandrasekhar [22] we are able to obtain an implicit series solution. This solution is valid for small values of the Frank-Kamenetskii parameter δ and positive values of the shape factor k.

7.1 Introduction

In Chapter 3 [52] we showed how a Lie symmetry reduction of the Lane-Emden equation (7.1) solved subject to $y(0) = y'(0) = 0$ can be used to obtain an implicit series solution that has a larger radius of convergence than a straightforward power series solution. The equation we considered modelled a process in a spherical vessel, i.e. had a shape factor of two. In this Chapter we consider a Lane-Emden equation with arbitrary shape factor with the same goal in mind. We consider the following equation

$$y'' + \frac{k}{x}y' + \delta e^y = 0 \tag{7.1}$$

which is a subclass of the generalised Lane-Emden equation of the second-kind given by [16]

$$y'' + \frac{\alpha}{x}y' + \beta x^{\nu-1}e^{ny} = 0 \tag{7.2}$$

where $' = d/dx$. The constants α, β, ν and n are determined from the physics of the problem under investigation. The model equation (7.1) is solved subject to the boundary conditions

$$y'(0) = 0, \qquad y(1) = 0 \tag{7.3}$$

as discussed in Chapter 2 when we considered the geometry of a cylindrical vessel.

Without recourse to the Lie group method we find an implicit series solution to equation (7.1). This solution is valid for positive shape factors and suitably small values of the critical value. This is shown through a comparison with a numerical solution obtained to the problem in question. The domain upon which the solution converges is not larger than the straightforward power series solution.

7.2 Power series solution

A straightforward power series solution of the form

$$y = \sum_{i=0}^{\infty} b_i x^i \tag{7.4}$$

admitted by (7.1) can easily be obtained by substituting (7.4) into (7.1) and separating by coefficients of powers of x. This is done by writing the following

$$y'(x) = \sum_{i=0}^{\infty} i b_i x^{i-1} \qquad y''(x) = \sum_{i=0}^{\infty} i^2 b_i x^{i-2} \tag{7.5}$$

and substituting into equation (7.1) to obtain

$$\sum_{i=0}^{\infty} i^2 b_i x^{i-2} + \sum_{i=0}^{\infty} k i^2 b_i x^{i-2} + \delta e^{\sum_{i=0}^{\infty} b_i x^i} = 0. \tag{7.6}$$

We expand and approximate the exponential term to find the following equation

$$\sum_{i=0}^{\infty} \left(i^2 b_i x^{i-2} + k i^2 b_i x^{i-2} + \delta(1 + \sum_{i=0}^{\infty} b_i x^i + \cdots) \right) = 0 \tag{7.7}$$

which by separating coefficients for different powers of x produces the values given by (7.8) - (7.11). Imposing the boundary condition $y'(0) = 0$ yields $b_1 = 0$. A consequence of $b_1 = 0$ is that all odd coefficients are zero, i.e. $b_{2i+1} = 0$, $i = 0, 1, 2, \ldots$. The first few terms of the even power series solution are given by

$$b_2 = -\frac{\delta e^{b_0}}{2(k+1)}, \tag{7.8}$$

$$b_4 = \frac{\delta^2 e^{2b_0}}{8(k+1)(k+3)}, \tag{7.9}$$

$$b_6 = -\frac{\delta^3 e^{3b_0}(k+2)}{24(k+1)^2(k+3)(k+5)}, \tag{7.10}$$

$$b_8 = \frac{\delta^4 e^{4b_0}(17 + k(16+3k))}{192(k+1)^3(k+3)(k+5)(k+7)}. \tag{7.11}$$

Imposing the boundary condition $y(1) = 0$ we obtain the nonlinear equation

$$\sum_{i=0}^{\infty} b_{2i} = 0 \tag{7.12}$$

that needs to be solved for b_0. The sequence of coefficients b_n is alternating with the term e^{b_0} always positive. As done in Chapter 3 we investigate the convergence of the power series (7.4) by considering the ratio test

$$\lim_{n\to\infty} \left| \frac{b_{2n+2} x^{2n+2}}{b_{2n} x^{2n}} \right|$$

$$= x^2 \lim_{n\to\infty} \left| \frac{b_{2n+2}}{b_{2n}} \right|. \tag{7.13}$$

The series of inequalities

$$\left| \frac{b_4}{b_2} \right| < \left| \frac{b_6}{b_4} \right| < \left| \frac{b_8}{b_6} \right| < \cdots < \left| \frac{b_{j+2}}{b_j} \right| < \cdots \tag{7.14}$$

is maintained for positive values of k and δ. The term e^{b_0} is to be observed in every coefficient b_n and is removed through division in (7.14). From (7.14) we find that in order for us to maintain convergence we require that $|x^2| < 1$ and since the power series solution (7.4) is even we find that it is valid on the domain

$$|x| < 1. \tag{7.15}$$

For more detail on this process refer to Sections 3.2 and 3.4, [41, 57].

From (7.15) we can conclude that the straightforward power series solution (7.4) is not valid on the domain on which the problem is specified. We aim to improve upon the power series solution (7.4) by using an appropriate set of coordinate transformations in the next Section.

7.3 Reduction to first-order

Transforming the coordinates of equation (7.1) using the transformations proposed by Chandrasekhar [22]

$$x = e^{\xi}, \qquad y = z - 2\xi \tag{7.16}$$

reduces (7.1) to the autonomous equation

$$z'' + (k-1)z' - 2(k-1) + \delta e^z = 0 \tag{7.17}$$

where $' = d/d\xi$. Making the substitution

$$z' = w(z), \qquad z'' = w\frac{dw}{dz} \tag{7.18}$$

reduces (7.17) to the Abel equation of the second-kind

$$\frac{1}{2}\frac{d(w^2)}{dz} + (k-1)w - 2(k-1) + \delta e^z = 0. \tag{7.19}$$

Equation (7.19) admits a power series solution

$$w = \sum_{j=0}^{\infty} a_j e^{jz}. \tag{7.20}$$

Using this power series solution and the fact that $w^2 = \sum_{j=0}^{\infty}\left(\sum_{i=0}^{j} a_i a_{j-i}\right) e^{jz}$ we are able to obtain the following coefficient values

$$a_0 = 2, \qquad a_1 = -\frac{\delta}{1+k}, \tag{7.21}$$

$$\frac{1}{2}j\left(\sum_{i=0}^{j} a_i a_{j-i}\right) + (k-1)a_j = 0, \qquad j = 2, 3, \ldots. \tag{7.22}$$

after appropriate substitutions into equation (7.19). Considering the power series (7.20) yields

$$a_j = -\frac{\frac{1}{2}j\sum_{i=1}^{j-1} a_i a_{j-i}}{ja_0 + k - 1}, \qquad j = 2, 3, \ldots. \tag{7.23}$$

leading to some of the following evaluations of (7.23)

$$a_2 = -\frac{\delta^2}{(1+k)^2(3+k)}, \tag{7.24}$$

$$a_3 = -\frac{3\delta^3}{(1+k)^3(3+k)(5+k)}, \tag{7.25}$$

$$a_4 = -\frac{2\delta^4(23+7k)}{(1+k)^4(3+k)^2(5+k)(7+k)}, \tag{7.26}$$

$$a_5 = -\frac{5\delta^5(67+17k)}{(1+k)^5(3+k)^2(5+k)(7+k)(9+k)}. \tag{7.27}$$

To ascertain the convergence of the power series solution (7.20) we need to ensure that the series of coefficients is decreasing. It can easily be proved that the above limit is maintained if we order the terms in an increasing sequence given by

$$|a_0| > |a_1| > |a_2| > \cdots > |a_j| > \cdots \tag{7.28}$$

From this sequence we have that

$$1 > \left|\frac{a_1}{a_0}\right| > \left|\frac{a_2}{a_1}\right| > \left|\frac{a_3}{a_2}\right| > \cdots > \left|\frac{a_{j+1}}{a_j}\right| > \cdots \tag{7.29}$$

which indicates that the coefficients will not hinder the capacity of the power series solution (7.20) to converge if (7.28) holds. In fact we find that (7.28) holds true for

$$0 < \delta < 1, \qquad k > 0 \tag{7.30}$$

confirming the fact that the coefficients are of a decreasing order as required for convergence.

In turn, from the ratio test, we can maintain that the power series (7.20) is valid on the domain

$$|e^z| < 1 \tag{7.31}$$

given the boundary conditions (7.3) which the equation (7.1) is subject to and the fact that the condition (7.30) holds. From (7.16) the domain of convergence in terms of the original variables is given by

$$\left|x^2 e^y\right| < 1. \tag{7.32}$$

At the boundary of the vessel where the boundary condition $y(1) = 0$ holds we find that $z = 0$. Hence the radius of convergence given by (7.31) seems reasonable showing that the power series (7.20) does indeed converge.

From (7.18) we obtain the first-order ordinary differential equation

$$\frac{dz}{d\xi} = \sum_{j=0}^{\infty} a_j e^{jz}. \tag{7.33}$$

From (7.16) the first-order ordinary differential equation (7.33) reduces to

$$x\frac{dy}{dx} + 2 = \sum_{j=0}^{\infty} a_j x^{2j} e^{jy}. \tag{7.34}$$

By defining

$$y^* = \ln\left(x^2 e^y\right) \tag{7.35}$$

the first-order ordinary differential equation (7.34) reduces to

$$x\frac{dy^*}{dx} = \sum_{j=0}^{\infty} a_j e^{jy^*}. \tag{7.36}$$

This is the same form as the first-order ordinary differential equation derived in Chapter 3 [52]. From there an approximate solution to the first-order ordinary differential equation (7.36) is given by

$$\ln x + \alpha = \frac{y^*}{a_0} - \sum_{j=1}^{m} \frac{a_j}{ja_0^2}\, e^{jy^*} \tag{7.37}$$

where α is a constant of integration and m an integer. Details of this calculation are presented in Chapter 3 [52] and are not repeated here. Substituting (7.35) into (7.37) and imposing $y(1) = 0$ from (7.3) we find that

$$\ln x\left(1 - \frac{2}{a_0}\right) - \sum_{j=1}^{m} \frac{a_j}{ja_0^2} = \frac{y}{a_0} - \sum_{j=1}^{m} \frac{a_j}{ja_0^2}\, x^{2j} e^{jy}. \tag{7.38}$$

Imposing $a_0 = 2$ on (7.38) we find that

$$y - \sum_{j=1}^{m} \frac{a_j}{2j}\, x^{2j} e^{jy} = -\sum_{j=1}^{m} \frac{a_j}{2j}. \tag{7.39}$$

As done in Chapter 3 [52] we substitute $y = \ln(1/x^2)$ into (7.39) to find that $x = 1$. This indicates that we were not able to improve the radius of convergence for the power series solution (7.4) as was done in Chapter 3 [52] for a shape factor of two. This seems reasonable when we consider the conditions (7.30) required for the validity of the implicit solution (7.39). In Chapter 3 [52] the parameter δ was one and hence not within the required interval for the implicit solution to be valid. This means that we can not equate the solutions in the hope of validating an improved domain of convergence.

The implicit equation (7.39) is easily solved by selecting values of k and δ that satisfy (7.30). Values of x are specified in the interval $[0, 1]$ and the resulting nonlinear equation solved for the corresponding values of y. We use the `FindRoot` routine in MATHEMATICA to solve the nonlinear equation (7.39).

We compare solutions of (7.39) with the case for which analytical solutions exist when $0 < \delta < 1$ and $k > 0$. As discussed in Chapter 2 when $k = 1$ (7.1) reduces to

$$y'' + \frac{y'}{x} + \delta e^y = 0. \tag{7.40}$$

Frank-Kamenetzkii [29, 21, 25] has found two solutions admitted by (7.40) given by

$$y = \log\left[\frac{16e^{c_1}}{(2\delta + e^{c_1}x^2)^2}\right], \qquad y = \log\left[\frac{16e^{c_2}}{(1 + 2\delta e^{c_2}x^2)^2}\right]. \tag{7.41}$$

The solutions from (7.41) satisfy the boundary condition $y'(0) = 0$. Imposing the boundary condition $y(1) = 0$ we obtain the two solutions

$$y = \log\left[\frac{8\left(-4 + 2\sqrt{4-2\delta} + \delta\right)}{\left(2\left(-2 + \sqrt{4-2\delta}\right)x^2 + \delta\left(x^2 - 1\right)\right)^2}\right], \qquad \delta \leq 2 \tag{7.42}$$

and

$$y = \log\left[\frac{8\left(4 + 2\sqrt{4-2\delta} - \delta\right)}{\left(-2\left(2 + \sqrt{4-2\delta}\right)x^2 + \delta\left(x^2 - 1\right)\right)^2}\right], \qquad \delta \leq 2. \tag{7.43}$$

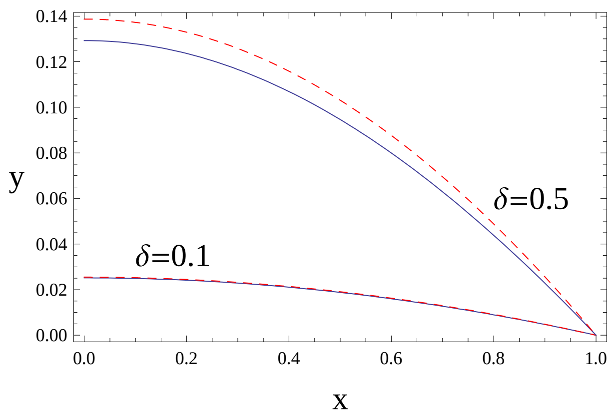

Figure 7.1: *Plot of the implicit series solution (7.39) for $k = 1$ where $m = 8$ and (7.42) $(- - -)$.*

From Figure 7.1 we observe that the approximate implicit solution (7.39) compares well with the analytical solution (7.42) for small values of δ. In the next Section we compare the approximate implicit solution (7.39) with numerical approximations of solutions to (7.1).

7.4 Comparison with a numerical solution

The model equation (7.1) is singular on the line $x = 0$. We approximate (7.1) at $x = 0$ by

$$y''(1+k) + \delta e^y = 0, \tag{7.44}$$

as discussed in Section 5.4. Hence we solve the system

$$y'' = \begin{cases} -\frac{\delta}{1+k} e^y, & x = 0, \\ -\frac{k}{x} y' - \delta e^y, & x \neq 0. \end{cases} \tag{7.45}$$

We divide the interval $[0, 1]$ up into $n+1$ equidistant points $x_{i+1} = x_i + h$ such that

$$0 = x_0 < x_1 < x_2 < \ldots < x_{n-1} < x_n = 1. \tag{7.46}$$

We use the notational convention $y_i = y(x_i)$. Derivatives are approximated at x_i by the central differences

$$y'(x_i) \approx \frac{y_{i+1} - y_{i-1}}{2h}, \qquad y''(x_i) \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}. \tag{7.47}$$

The boundary conditions (7.3) imply that

$$y_{-1} = y_1, \qquad y_n = 0. \tag{7.48}$$

The resulting nonlinear system of equations we have to solve is given by

$$\begin{bmatrix} -2 & 2 & 0 & 0 & \ldots & 0 & 0 & 0 \\ \alpha_1 & -2 & \beta_1 & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \alpha_2 & -2 & \beta_2 & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \alpha_{n-1} & -2 & \beta_{n-1} \\ 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{n-1} \\ y_n \end{bmatrix} = -\delta h^2 \begin{bmatrix} \frac{1}{(1+k)} e^{y_0} \\ e^{y_1} \\ e^{y_2} \\ \vdots \\ e^{y_{n-1}} \\ 0 \end{bmatrix} \tag{7.49}$$

where

$$\alpha_i = \left(1 - \frac{kh}{2x_i}\right), \qquad \beta_i = \left(1 + \frac{kh}{2x_i}\right). \tag{7.50}$$

The system (7.49) is reduced to the linear system by writing it as

$$\begin{bmatrix} -2 & 2 & 0 & 0 & \dots & 0 & 0 & 0 \\ \alpha_1 & -2 & \beta_1 & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \alpha_2 & -2 & \beta_2 & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \alpha_{n-1} & -2 & \beta_{n-1} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y_0^{(i+1)} \\ y_1^{(i+1)} \\ y_2^{(i+1)} \\ \vdots \\ \vdots \\ y_{n-1}^{(i+1)} \\ y_n^{(i+1)} \end{bmatrix} = -\delta h^2 \begin{bmatrix} \frac{1}{(1+k)} e^{y_0^{(i)}} \\ e^{y_1^{(i)}} \\ e^{y_2^{(i)}} \\ \vdots \\ \vdots \\ e^{y_{n-1}^{(i)}} \\ 0 \end{bmatrix} \tag{7.51}$$

where we assume an initial $\mathbf{y}$ vector with components given by

$$y_i^{(0)} = \frac{k}{2}\left(1 - x_i^2\right). \tag{7.52}$$

The system (7.51) was presented in Chapter 5 [36]. The initial guess (7.52) has been shown in Section 5.6 [38] to be appropriate to avoid the instabilities mentioned in Chapter 5 [36].

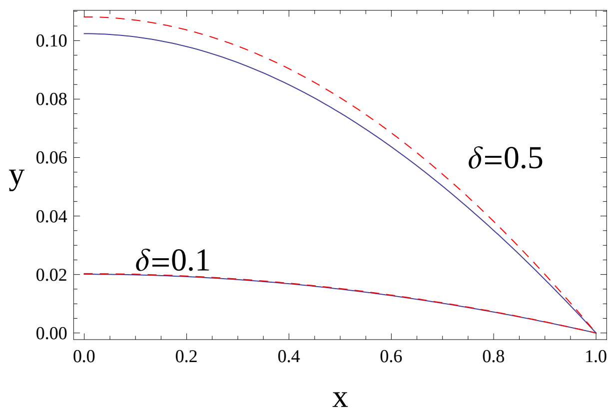

Figure 7.2: *Plot of the implicit series solution (7.39) for $k = 1.5$ where $m = 8$ and a numerical solution obtained by iterating the system (7.51) $(- - -)$.*

In Figure 7.2 we plot a numerical solution admitted by (7.1) by iterating the linear system (7.51) and the approximate implicit solution (7.39). Once again we note that the approximate implicit solution compares well with the numerical solution for small values of δ.

7.5 Concluding remarks

The implicit series solution (7.42) has been found without a recourse to Lie group theory as in the case investigated in Chapter 3 [52]. By comparing the approximate implicit solution (7.42) with an analytical solution (7.42) valid for $k = 1$ and a numerical solution obtained using finite differences we have shown that (7.42) is valid for small values of the Frank-Kamenetskii parameter δ and for positive values of the shape constant k.

The implicit series solution does not have a larger radius of convergence when compared to the straightforward power series solution. This does not contradict the improved domain of convergence found for $k = 2$ in Chapter 3 [52] since the requirement that $0 < \delta < 1$ was not met for the relevant problem. We have shown that for the initial value problem $y(0) = y'(0) = 0$, discussed in Chapter 3 [52], we get a radius of convergence greater than one. In this Chapter we have applied the same technique to the Lane-Emden equation (7.1) subject to the boundary conditions given by $y'(0) = 0$ and $y(1) = 0$. The domain of the boundary value problem we considered is $x \in [0, 1]$. Since a typical power series converges for $|x| < 1$, as we have shown, and our implicit solution has a radius of convergence $|x| > 1$ we can say that our implicit series solution (7.39) to the boundary value problem is more accurate.

The advantage of using this approach is the ease with which the boundary conditions could be imposed when compared to a straightforward power series solution. The approximate power series solution obtained using this approach provides a useful comparison to the numerical solutions obtained.

Chapter 8

Conclusion

The Lane-Emden equation of the second-kind investigated in this thesis was considered for its capacity to model two physical processes. One such process occurs within the field of astronomy. In this context the equation models the dimensionless density distribution of an isothermal gas sphere. The equation may also be transformed into equations modeling Richardson's theory of thermionic currents [58] and Bonnor-Ebert gas spheres [15]. The second model considered with particular emphasis originates within ignition theory. The model describes the steady state temperature distribution within a vessel. An important consideration within our investigations is that the stationary distribution in the reacting system becomes impossible at some critical condition. A parameter δ is associated with this critical condition and can be useful to obtain. The value of δ, also known as the Frank-Kamenetskii parameter [29], can be shown to be dependent on the boundary conditions of the vessel. The geometry of the vessel modelled by the equation is specified by the parameter k known as the shape factor.

8.1 Applications of Lie group theory

8.1.1 Lie group method and Non-local symmetries

In the pursuit of an analytical solution to the equation modelling the dimensionless density distribution of an isothermal gas sphere we used the powerful technique of Lie group analysis and power series to determine a new approximate implicit solution admitted by the Lane-Emden equation. Obtaining an infinitesimal generator enabled us to find differential invariants which were used to reduce the order of the equation. Through an appropriate transformation we obtained an Abel equation of the second-kind which admitted a power series solution. By imposing the relevant condition and converting to the original variables we obtained an approximate implicit solution admitted by the original Lane-Emden equation. This new solution has a larger radius of convergence than the straightforward power series solution. Though the improvement may at first seem minor, it must be noted that the improvement was obtained while considering a non-dimensional equation. The actual improvement, in terms of the proper dimensions, would be much larger. The approach taken to obtain a new approximate implicit solution admitted by the Lane-Emden equation of the second-kind can be used to determine approximate solutions for ordinary differential equations that admit Lie point symmetries. This is a useful and powerful technique as one can obtain solutions valid over larger domains.

Steady state solutions for a thermal explosion in a cylindrical vessel have been obtained by Frank-Kamenetskii [29]. Our approach was unique in the sense that we observed the combustion behaviour of the model by considering the differential equation and not by solving the partial differential equation. We were able to find the solution obtained by Frank-Kamenetskii [29] which models the steady state temperature distribution. The Lie group method was used to obtain a new parametric solution. The parametric solution we have obtained is not physical in terms of the model considered. Considering a non-local symmetry found using the algorithm from Adam and Mahomed [2, 3] a singular imaginary solution was found. The solution obtained from the non-local symmetry approach is a new solution describing the ignition phenomenon. In order to ascertain the physical significance of the steady state solution obtained by Frank-Kamenetskii [29] and the imaginary solution obtained in this thesis using a non-local symmetry we considered similarity solutions of the Lane-Emden equation, hence taking into account the dependence of time. We discovered that the steady state solution is valid one step before ignition. Whereas the imaginary solution obtained from a non-local symmetry models the steady state solution one time step after ignition. Having plotted these solutions we see that they both decrease at the same gradient over time, indicating the diminishing temperature after combustion. The imaginary solution is singular after ignition, which in turn is indicative of the ignition represented by this solution. Separating the solution y into an imaginary and real solution, $y = y_0 + \imath y_1$, we observed the possibility that when combustion occurs there is an imaginary coordinate transformation taking place. This was supported by the fact that a real solution had been found to model the solution one time step before ignition and an imaginary solution one time step after ignition. Future work will be pursued considering this transformation into an imaginary coordinate system, and other aspects concerning the combustion occurring in this model.

The Lie group method was useful in obtaining invariant boundary conditions admitted by the Lane-Emden equation of the second-kind. To be able to apply numerical methods to the system it was important to do a dynamical stability analysis of the system first so that we may solve the resulting boundary value problem. The invariant boundary conditions were used in our analysis, where the shape factor and critical value remained arbitrary, as the conditions for the first-order autonomous system considered. We note that the stability of the boundary condition $y' = 0$ on $x = 0$ changes from stable for shape factor $k > 1$ to unstable for $k \leq 1$. These invariant boundary conditions were also used to obtain a solution dependent on the critical condition value for the case $k = 1$.

8.1.2 Noether's Theorem

We have used Noether's theorem [53] to determine first integrals of the Lane-Emden equation of the second-kind with arbitrary shape factor and critical value, δ. By applying the boundary conditions on these first integrals we found relationships between the the critical value and the boundary conditions of the vessel. We found that the temperature gradient at the boundary walls is symmetric within a rectangular geometry, $k = 0$. We used this physical symmetry by imposing the boundary conditions that correspond to the cylindrical geometry case. In this way we showed how the temperature at the centre of the rectangular vessel can be controlled by modifying the temperature gradient at the walls of the rectangular vessel. Two new boundary conditions that can be used to solve the equation in question for $k = 0$ were obtained. For the case $k = 1$, a cylindrical geometry, we showed how the critical value of $\delta = 2$ can easily be obtained without recourse to a solution of the problem. Future work involves applying the approach presented here to other boundary value problems.

In order to investigate the occurrence of multiple values at the boundaries of the Lane-Emden equation of the second-kind we investigated approximate first integrals admitted by the perturbed Lane-Emden equation. These first integrals were obtained through the application of Noether's theorem [53]. The equation models a thermal explosion in a vessel with thermally conducting walls. It was found that the temperature at the center is positive because the chemical reaction is producing heat, i.e. $y(0) > 0$. The temperature at the centre of the vessel is always higher than the temperature at the walls. This implied that the temperature gradient at the walls is always negative, i.e. $y'(1) < 0$. Relationships between the critical value, the boundary conditions and the perturbation element ϵ were found, indicating multiple values at the boundaries. For the case $k = 0$ we note that with $\epsilon = 0$ no multiple values occurred at the boundaries whereas for $\epsilon \neq 0$ we observed the presence thereof. Considering a numerical solution of the equation for $k = 0$ we discovered that for a fixed temperature gradient at the rectangular vessel walls we get two possible values for the temperature at the center of the rectangular vessel, i.e. there are two values of $y(0)$ that satisfy the physical boundary condition $y'(0) = 0$. However there is only one value of $y'(1)$ that corresponds to $y(1) = 0$. Multiple values of $y(0)$ exist for a fixed value of $y'(1)$ for small ϵ. The case $k = 1$ exhibited similar results for small values of ϵ. Multiple values of $y'(1)$ exist for fixed values of $y(0)$. Future research involves applying the techniques developed here to other physical problems to see if further insights can be gained by investigating approximate first integrals admitted by the model equations.

8.2 Numerical analysis

In Section 8.1.1 we discussed how through the use of infinitesimal transformations and invariant solutions we were able to obtain an approximate implicit series solution. However it is computationally more expensive to determine the new approximate implicit solution. In order to overcome this we specified y-values and solved the equation for x. The divergence of the approximate implicit solution away from the power series solution is a new phenomenon. This has lead us to conclude that the divergence is not a numerical phenomenon. The approximate implicit solution has a larger radius of convergence when compared with the power series solution. This is useful provided the ratio ρ/ρ_c is within the limits of stability for the isothermal gas sphere under consideration as was the case here. We have also found that this lower bound ratio for the new approximate implicit solution is larger than that of the original power series solution. The ratio ρ/ρ_c for both the power series solution and the approximate implicit solution does not diverge as much as the different solutions do.

We also considered a linearized version of the Lane-Emden equation of the second-kind valid on a small interval $x \in [0, x^* \ll 1]$ about the center of a cylinder. This equation was used to approximate the thermal explosion problem. A numerical solution is obtained using non-local symmetries to provide an initial guess for the boundary value problem solver in MATLAB. This numerical solution has a higher maximum temperature and a lower activation energy for the critical values in the theory of thermal explosions. And so if the activation energy of a particular chemical reaction is lower and the dimensions of the cylindrical vessel remain the same then the chemical reaction will attain a higher maximum temperature. Future work will involve investigating the effects of convection on the temperature distribution in the cylindrical vessel.

Considering a similar linearized form of the Lane-Emden equation as mentioned in the above paragraph, modelling the thermal explosion problem, we obtained a consistency criteria that must be maintained by any numerical scheme used. The criteria is dependent on the shape factor and critical value, both of which are defined to be arbitrary constants. We solved the boundary value problem by first choosing initial guesses to the initial height and gradient of the temperature in the vessel. Then as suggested in Shampine [61] we chose a suitable initial function as a guess. However both approaches still revealed solutions indicating the presence of the instability of $y' = 0$ and $x = 0$ discussed in Section 8.1.1. This may be due to the fact that the initial guess that we have chosen is a polynomial while analytical solutions obtained by Frank-Kamenetskii [29] and Chambré [21] are logarithmic. We showed that this instability does not manifest when solving an initial value problem within an infinite slab. We were able to overcome the instability by using a central difference approximation to the derivatives in our model equation. The occurrence of this instability is not obvious indicating that the method of central differences is able to overcome it. Analytically we are able to calculate approximate guesses for the values of $k \ll 1$ and $\frac{1}{k} \ll 1$. We do this by assuming that the solution has the form of a power series under the assumption that $\delta = O(k)$. This process is followed revealing solutions valid over two separate domains: for large values of k and small values of k. And so we were able to find approximate solutions, to be used as initial guesses, that are able to overcome the instability of the boundary condition $y'(0) = 0$ for $k \leq 1$.

A solution to the Lane-Emden equation without specifying the values of the shape factor or critical condition was found. This solution was found without recourse to Lie point symmetries but by using transformations proposed by Chandrasekhar [22]. We considered a linearized version of the Lane-Emden equation and approximated the system of equations via central differences. From here we were able to obtain a numerical solution which we compared with the approximate implicit solution found and an analytical solution that is valid for $k = 1$. In this way we showed that the implicit series solution is valid for small values of the Frank-Kamenetskii [29] parameter δ and for positive values of the shape constant k. The advantage of using this approach is the ease with which the boundary conditions could be imposed which is not the case with a straightforward power series solution. The implicit series solution does not have a larger radius of convergence when compared to a straightforward power series solution. This may seem inconsistent with the results obtained for the Lane-Emden equation describing the dimensionless density distribution in an isothermal sphere where we obtained an approximate implicit solution with a larger radius of convergence than than the power series solution. However, though $k = 2$ and hence positive, the critical value was not suitably small for the implicit series solution to be valid. For the approximate implicit solution obtained the value of δ was one which is not within the range required for the implicit series solution to be valid. The domain of the boundary value problem for which we obtained the implicit series solution is $x \in [0, 1]$. We claim that our solution to the boundary value problem is more accurate since the implicit series solution has a radius of convergence $|x| > 1$.

8.3 Final note

In this thesis our aim was to find an analytical solution to a generalised form of a Lane-Emden equation of the second-kind where in particular the shape factor and critical value were left arbitrary. Though we were unable to do so we were able to find new solutions for the geometry of an infinite slab, infinite circular cylinder and sphere. For positive shape factors and suitably small values of the critical value we were able to find an implicit series solution to the Lane-Emden equation considered. These solutions, along with the various approximate solutions found, provided great insight into the Lane-Emden equation of the second-kind and the physical processes it models. The relationships found between the critical value and boundary conditions provided us with two new boundary conditions valid for the equation under a specified shape factor. In this way the value of the critical condition was also obtained without recourse to a solution of the problem. We were also able to obtain new invariant boundary conditions which enabled us to to a dynamical systems analysis. This allowed us to make predictions concerning the properties of the solutions of the equation providing new insights into the stability of the boundary conditions.

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